Non-adiabatic Berry phases for periodic Hamiltonians

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Abstract

A method for the calculation of Berry phases for periodic, but not necessarily adiabatic, Hamiltonians is reported. This method is based on a novel factorisation of the evolution operator and is in the spirit of the theory of systems of linear differential equations with periodic coefficients.

The use of this approach in practical situations is greatly facilitated by exploiting the Fourier decomposition of the Hamiltonian. This converts the problem into an equivalent time-independent form. The solution to the problem is then expressible in terms of the eigenvectors and eigenvalues of a certain self-adjoint operator called the Floquet Hamiltonian. This operator can be calculated from the Fourier decomposition of the original Hamiltonian.

Our formalism has several calculational advantages over the other methods used in the literature. These advantages are best seen by considering standard quantum optical systems such as the semi-classical model of a two-level atom strongly irradiated by a near resonant laser beam. The utility of our formalism is not confined to systems of this type however. For example it can be used to great advantage in the study of systems with time-odd electron-phonon coupling.

Apart from its calculational utility, our formalism also has important theoretical applications. Here it is used to clarify the relationship between Berry phases and the time dependence of the Hamiltonian.

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Contents

Chapter One

Introduction

In quantum mechanics, a state is described by a ket in some Hilbert space. For example, the state of a single non-relativistic particle is a complex-valued function of the spatial variables. However this mathematical description contains a redundancy. Two wavefunctions ϕ_1 and ϕ_2 that differ by only a multiplicative phase (that is $\phi_2 = \exp\{i\theta\}\phi_1$) represent the same isolated state. This is the origin of the statement that quantum mechanics contains an arbitrary phase.

This might lead one to think that the phase of a wavefunction is irrelevant. However this is not true for the following reason. The above states ϕ_1 and ϕ_2 are only the same in isolation. When they are made to interact with some other state, it is possible to gain some information on their phase difference. Informally, considered in isolation, the two states which will be made to interfere each have an arbitrary phase. However when they are actually interacting, the joint system has only a single arbitrary phase and so their phase difference must be measurable.

As a very simple example of this, imagine that the initial and final states of an evolving system were equal up to a multiplicative phase: $\phi(\tilde{t}) = \exp\{i\chi\}\phi(0)$. In future I will call such an initial state a cyclic initial state. Now imagine that we prepared two copies of the intial state $\phi(0)$ and kept one of them constant throughout the evolution of the other. Then at time $\tilde{t}$ the phase difference χ is measurable by direct interference.

As we now know that the evolving phase of a quantum system is measurable, it is important to try to understand its physical significance. That is we want to be able to calculate it and understand its origin. It turns out that this overall phase χ is most naturally desribed as the sum of two parts. The first, called the

dynamical phase, is a measure of the length of time for which the system has been evolving. The remainder, called the Berry phase, is a measure of where the system has been.

Hence the dynamical phase comes from the dynamical aspect of the evolution whereas the Berry phase is geometric in origin. This last fact has lead many authors, including Berry himself, to name the Berry phase the geometrical phase.

One of the most intuitive examples of the Berry phase arises in the adiabatic theorem [Berry 1984]. The adiabatic theorem states that a slowly driven system will respond by following the eigenspaces of the time-dependent Hamiltonian. Now if we drive the parameters upon which the Hamiltonian depends around a closed path, the initial and final eigenspaces are the same. Hence if the system is non-degenerate, the initial eigenstates are cyclic initial states.

It turns out that in this example the dynamical phase has a particularly simple form, being just the time integral of the instantaneous energy around the circuit. Hence the dynamical phase can be thought of as a naive generalisation of the evolving phase in the time-independent case. This interpretation has a natural extension to the non-adiabatic case, with the instantaneous energy being replaced by the instantaneous expectation value of the Hamiltonian. Thus we see that the dynamical phase depends on the "energy" of the system and the time taken for its evolution. This contrats with the Berry phase, which only depends on the geometry of the evolution [Simon 1983].

An important ramification of the existence of the adiabatic Berry phase is in the Born-Oppenheimer approximation. Here Berry phases lead to the presence of an extra vector potential in the effective Hamiltonian for the slow degrees of freedom [Mead 1987, Kuratsuji and Iida 1985]. This potential has proven to be important in, among other things, the study of slow atomic collisions [Zygelman 1987] and field theoretic anomalies [Nelson and Alvarez-Guamé 1985, Semenoff 1986].

It is important to note that several aspects of the Berry phase were known before Berry's seminal paper. For example, Berry [1984] notes that the effect of

adiabatic phases in the Born-Oppenheimer approximation had been anticipated by Mead [Mead and Truhlar 1979], the latter authors describing it as the "molecular Aharonov-Bohm effect". Berry [1987] also notes that a generalised form of the Berry phase was discussed in the context of the interference of light beams as early as 1956 [Pancharatnam 1956]. Further examples of the prehistory of Berry phase are given by Berry [1990b]

Since the discovery of the Berry phase, there have been many experimental verifications of its existence. For instance, Berry phases may be directly measured by passing a linearly polarised laser down a helically wound optical fibre [Chiao and Wu 1986, Tomita and Chiao 1986]. Here the Berry phase is manifested as the rotation of the plane of polarisation of the laser as it travels down the fibre. The Berry phases that arise when a circularly polarised laser is used (as in the example on page two) are also easily measured [Chiao and Wu 1986]. Here two counter-rotating fibres are used. This is because the dynamical phases for the two fibres are the same, while the Berry phases differ by a sign. Hence the interference of the two output beams gives the Berry phase. Other experiments include neutron interferometry [Wagh and Rakhecha 1990] and electron diffraction from a screw dislocation [Bird and Preston 1988].

The Berry phase has also been used to explain previously known phenomena. For example, it can be used to interpret the Mollow triplet splitting [Moore 1990b] and the sequence of states in the $E \otimes \epsilon$ Jahn-Teller problem [Ham 1987]. Other cases include the Sagnac effect [Hendricks and Nienhuis 1990] and quantum interference in general rotating systems [Xu and Tsai 1990].

Finally there have been many reviews and books on the Berry phase. Some of the most important of these are Shapere and Wilczek [1989], Jackiw [1988], Zwanziger *et al.* [1990] and Morkovski and Vinitsky [1989].

My contribution to the study of Berry phases has involved the creation of an operator decomposition scheme for the calculation of non-adiabatic Berry phases for periodic Hamiltonians. Here the evolution operator U is written as the product

$$U(t) = Z(t)\mathrm{e}^{\mathrm{i}Mt}. \tag{1.1}$$

$Z(t)$ is constrained to be periodic and unitary, while M is constant and self-adjoint. This leads to the identification of the cyclic initial states $\phi_\alpha(0)$ as the eigenvectors of M, with the corresponding Berry phases being given by

$$\gamma_\alpha = \mathrm{i}\int_0^{\tilde{t}} \langle \phi_\alpha(0) \mid Z^*(t)\dot{Z}(t) \mid \phi_\alpha(0)\rangle \, \mathrm{d}t. \tag{1.2}$$

This approach is useful from a purely calculational standpoint as it allows one to exploit the Fourier decomposition of the (periodic) Hamiltonian. This leads to the identification of the cyclic initial states as the eigenvectors of the Floquet Hamiltonian

$$K = H(t) - \mathrm{i}\tfrac{\partial}{\partial t}. \tag{1.3}$$

The operator decomposition formalism also has many practical applications. For example, it allows one to interpret the Rabi oscillations and Mollow triplet splitting of quantum optics . Further, it leads to a modified adiabatic ansatz for systems with both adiabatic and non-adiabatic time dependence.

The rest of this thesis is organised as follows. In chapter 2 I discuss the origin of time dependence in quantum Hamiltonians. This is important as the Berry phases for time-dependent systems arise for very different reasons than those for time-independent ones. This fact is discussed in section 5.2. As chapter 2 is designed to provide some technical background, it can safely be ignored on the first reading.

In chapter 3 I define Berry phases and show how to calculate them in terms of single-valued vectors. These are vectors $\psi(t)$ which follow the evolving vector $\phi(t)$ up to a phase and have the property that $\psi(\tilde{t}) = \psi(0)$. As such, they are the non-adiabatic analogues of the instantaneous eigenvectors $\zeta(R(t))$ defined earlier. This calculational approach provides the basis for the methods developed in later chapters. The measurement of Berry phases is also discussed.

While my work has involved the non-adiabatic Berry phase, for completeness a brief discussion of the adiabatic case is given in chapter 4. Note that the importance of the adiabatic Berry phase is not merely historical. In fact, one of the

most important applications of Berry phase is in the Born-Oppenheimer approximation. This involves the adiabatic decoupling of fast degrees of freedom from a slowly varying background.

The body of my theoretical work is contained in chapters 5 and 6. In chapter 5 the operator decomposition of equation (1.3) is discussed. This leads to the notion of quasi-degeneracy, which helps to explain the relationship between the Berry phase and the time dependence of the Hamiltonian. By utilising the Fourier decomposition of the Hamiltonian, the results of the operator decomposition formalism can be recast into time-independent form. This is discussed in chapter 6.

There are two other main methods for the calculation of Berry phases, involving the geometric and algebraic properties of the quantum evolution respectively [Aharonov and Anandan 1987, Page 1987, Brihaye *et al.* 1990]. While I have not been directly involved in the development of either of these, for completeness they are discussed in chapter 7 from the perspective of my work.

Most papers on Berry phase tacitly assume that cyclic initial states exist. However as I show in chapter 8, this is not necessarily the case. While there is no general characterisation of which systems do have a complete set of such states, there are many useful partial results. I discuss the most important of these.

In chapters 9 and 10, I discuss the application of the operator decomposition scheme to quantum optical problems. This leads to the interpretation of the Rabi oscillations in terms of Berry phases and a method for the treatment of systems with both adiabatic and non-adiabatic time dependence.

Finally, in chapter 11 I summarise the extensions to the definition of Berry phase that have been reported in the literature so far. These include the treatment of non-cyclic evolution and mixed initial states.

For convenience, some of the technical results needed in this work are collected in appendices. Appendix A contains some mathematical preliminaries, including some simple functional analysis and a brief discussion of fibre bundles. These results are used to derive the evolution operator decomposition of section 5.1 and

are needed in section 7.1 for the discussion of the geometric interpretation of the Berry phase.

Further, in appendix B I summarise some of the properties of coherent states. These are used in section 2.1, where I derive the Hamiltonian of the semi-classical Jaynes-Cummings model, and section 8.2, where I derive necessary and sufficient conditions for the existence of cyclic initial states for the forced harmonic oscillator.

Appendix C contains a brief discussion of the effects of time-reversal odd coupling in ligand field theory. This study helps to explain, among other things, the effect of time reversal symmetry on the Berry phase. Finally, appendix D contains a glossary of the important technical terms used in this thesis.

Chapter Two

Time-dependent Hamiltonians

The existence of Berry phases is intimately linked to Hamiltonian time dependence. As I will show in section 5.2, Berry phases arise in time-independent systems for very different reasons than in time-dependent ones. However, it is well known that the Hamiltonian of an isolated system must be time-independent. Hence any time dependence must come from the interaction of the system with its surroundings. I will discuss this issue in some detail in this chapter. As this chapter is designed to provide a technical background for the work of later chapters it may be safely omitted on first reading.

In section 2.1 I discuss isolated systems. Here the existence of the evolution operator is guaranteed by Stone's theorem. This result also leads to the notion of stationary states. These are initial vectors that remain in the same physical state throughout their evolution, only picking up a time-dependent phase. In section 3.1, this idea will be generalised to periodic Hamiltonians, leading to the definition of Berry phase.

Having analysed the time-independent case, in section 2.2 I discuss interacting systems. Here the existence of the evolution operator is harder to prove, requiring additional constraints on the Hamiltonian [Avron *et al.* 1987, Yajima 1987]. While these constraints are highly technical and always met in practice, I include them for completeness. After discussing these, I explicitly show how the time-dependence of the semi-classical Jaynes-Cummings model arises. This uses the reduced density operator [Haake 1973] and follows the argument in Moore and Stedman [1990c].

This example is given for two reasons. First, it provides a system where the physical origins of time dependence are particularly clear. Hence we can verify that

the reduced density operator formalism does indeed give us the intuitive results that we expect. Second, I will often use the semi-classical Jaynes-Cummings model as an example. This is because its mathematical simplicity allows us to highlight the important features of our calculational scheme. This is discussed in chapters 5 and 6. Further, as I will show in section 9.1, it allows us to interpret the Berry phase in a physically meaningful way.

2.1 Isolated systems

As an isolated system has no non-conservative forces, its Hamiltonian H must be time-independent. Hence the time-dependent Schrödinger equation

$$\mathrm{i}\dot{U}(t) = HU(t) \tag{2.1}$$

has for its solution

$$U(t) = \exp\{-\mathrm{i}Ht\}. \tag{2.2}$$

Note that $U(0) = 1$ and $U(s)U(t) = U(t+s)$ for all t and s. Thus $U(t)$ is a strongly continuous one-parameter unitary group [Conway 1985, p336]. The fact that all such groups arise as the exponentials of anti-self-adjoint time-independent operators is known as Stone's theorem [Weidmann 1980, p222]. This is discussed in more detail in section A.1.

I now use the exponential representation of the evolution operator to establish the existence of stationary states. Let ζ be an eigenvector of H with energy E. Then using equation (2.2), we can write down the evolution of the initial state $\phi(0) = \zeta$, giving

$$\phi(t) = \mathrm{e}^{-\mathrm{i}Et}\zeta. \tag{2.3}$$

We call $\delta = -Et$ the *dynamical phase.*

Now vectors differing only by a phase are physically equivalent. Hence an initial eigenstate of a time-independent Hamiltonian stays in the same physical state

throughout its evolution. Such a vector is called a *stationary state* [Merzbacher 1970, p45]. In section 3.1, I show that the analogy of this behaviour in the time-dependent case leads to the definition of the Berry phase.

2.2 Interacting systems

To obtain Hamiltonian time dependence, we have to allow the system under study to interact with its surroundings. For example, consider an atom in an external magnetic field. By changing the direction of the magnetic field, we induce time dependence into the atomic Hamiltonian.

This can be compared to the breaking of time-reversal invariance. An isolated system must be time-reversal even. This restriction has many observable consequences. For example, in section 4.2, I show that it forces the Berry phases of an adiabatic system to be integral multiples of π. However, as I will discuss in appendix C, the interaction of the system with its surroundings can break this symmetry. The atomic system discussed in the last paragraph provides a good example, as a magnetic field is time-odd.

Mathematically, it is much harder to find the time evolution of time-dependent systems than it is for constant ones. To guarantee the existence of the evolution operator, we must constrain the Hamiltonian. There are many sets of sufficient conditions for the existence of dynamics. For example, it is sufficient that H have a time-independent closed domain, be bounded from below and be a twice continuously differentiable function of time [Avron *et al.* 1987].

If we take the Hilbert space to be $L^2(\mathbb{R}^n, \mathrm{d}^n x)$ then we can write the Hamiltonian in the form

$$H(t) = -\tfrac{1}{2}\nabla^2 + V(x,t) \tag{2.4}$$

for some function $V(x,t)$. The existence of the evolution operator then depends on the properties of V [Yajima 1987].

The way that interactions induce Hamiltonian time dependence is best seen by example. For the reasons listed in the introduction to this chapter, in the rest of

this thesis I will often use the semi-classical Jaynes-Cummings model. Physically, this model describes the interaction of a two-level atom with a semi-classical laser. For convenience I will assume that the laser is resonant with the atomic frequency. For this system, the time-dependence of the Hamiltonian derives from the semi-classical treatment of the laser.

The easiest way to see this is to use the reduced density operator formalism [Haake 1973]. We start with the quantum Jaynes-Cummings model, which contains both the electronic and photon degrees of freedom. As the quantum model describes an isolated system, the Hamiltonian is time-independent. Using equation (2.2) then gives the evolving density operator. However, we are only interested in the atomic degrees of freedom. To get rid of the photon states we merely trace over them. This gives a purely electronic density operator, called the *reduced density operator*. Finally, this is used to generate the semi-classical Hamiltonian. We find that it is indeed time-dependent.I follow Moore and Stedman [1990c].

Explicitly, the quantum Jaynes-Cummings model has the Hamiltonian [Jaynes and Cummings 1963]

$$H_j = \tfrac{\omega}{2}\sigma_z + \omega b^* b + \lambda(\sigma_+ b + \sigma_- b^*). \tag{2.5}$$

Here the σ's are electronic operators, b^* creates a photon in the cavity mode of interest and λ is a coupling constant. The j subscript indicates that this is the Hamiltonian of the joint electron-photon system.

Since H_j is time-independent, we can find the evolution of an arbitrary initial state by expressing it as a linear combination of the Hamiltonian's eigenstates and using equation (2.2). First we must decide on the initial state we wish to use. We want to extract the semi-classical electronic evolution, so it is natural to start in the product of an arbitrary electronic state $\phi(0)$ and a photon state $\Psi(0)$. Now the semi-classical laser is best described by a photon coherent state (see section B.2)

$$|\, z\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} |\, n\rangle. \tag{2.6}$$

Hence we take

$$\Phi(0) = \phi(0) \mid z\rangle. \tag{2.7}$$

We also assume that the laser is intense so that $|z|$ is large. Hence the Poisson distribution of number states in $\mid z\rangle$ is strongly peaked about $|z|^2$. The fact that the amplitude $z^n(n!)^{-1/2}$ is negligible for all n except those near $|z|^2$ has two effects. First, we may ignore the $n = 0$ term in the expansion (2.6). This is useful as the ground state has a different form to the rest of the eigenvectors of H_j and so ignoring it greatly simplifies the algebra. Second, it means that we can replace $\sqrt{n}$ by its mean value $|z|$. Thus we can replace terms of the form $z/\sqrt{n}$ by $\mathrm{e}^{\mathrm{i}\theta}$, where θ is the phase of z.

To solve the time-dependent Schrödinger equation, we must express $\Phi(0)$ as a linear combination of the eigenstates $\mid \epsilon_{\pm n}\rangle$ of H_j. By direct substitution, one can easily verify that these are given by

$$\mid \epsilon_{\pm n}\rangle = \sqrt{\tfrac{1}{2}} \mid +, n\rangle \pm \sqrt{\tfrac{1}{2}} \mid -, n+1\rangle. \tag{2.8}$$

The labels $\pm$ and n refer to the atomic state and photon number respectively. The corresponding eigenvalues are

$$\epsilon_{\pm n} = (n + \tfrac{1}{2})\omega \pm \lambda\sqrt{n+1}. \tag{2.9}$$

We ignore the ground state $\mid \epsilon_g\rangle$ with energy $-\omega/2$. This is possible as we assume that $|z|$ is large.

Let the initial electronic state have the form

$$\phi(0) = a_+ \mid +\rangle + a_- \mid -\rangle. \tag{2.10}$$

Then, substituting equations (2.10), (2.8) and (2.6) into equation (2.7), we find that the joint electron-photon initial state is given by

$$\Phi(0) = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} (a_+ \mid +, n\rangle + a- \mid -, n+1\rangle)$$

$$
\begin{aligned}
&= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \big(a_+ \big(\sqrt{\tfrac{1}{2}} \mid \epsilon_{+,n}\rangle + \sqrt{\tfrac{1}{2}} \mid \epsilon_{-,n}\rangle\big) \\
&\qquad + a_- \frac{z}{\sqrt{n+1}} \big(\sqrt{\tfrac{1}{2}} \mid \epsilon_{+,n}\rangle - \sqrt{\tfrac{1}{2}} \mid \epsilon_{-,n}\rangle\big)\big) \\
&= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \big(\sqrt{\tfrac{1}{2}} (a_+ + \mathrm{e}^{\mathrm{i}\theta} a_-) \mid \epsilon_{+,n}\rangle \\
&\qquad + \sqrt{\tfrac{1}{2}} (a_+ - \mathrm{e}^{\mathrm{i}\theta} a_-) \mid \epsilon_{-,n}\rangle\big). \qquad (2.11)
\end{aligned}
$$

Now as $|z|$ is large, the eigenvalues of H_j can be written as

$$\epsilon_{\pm n} = (n + \tfrac{1}{2})\omega \pm k, \qquad (2.12)$$

where the electronic coupling constant is given by $k = \lambda|z|$. Hence by applying equation (2.3), we find that the evolved state is given by

$$
\begin{aligned}
\Phi(t) &= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \big(\sqrt{\tfrac{1}{2}} (a_+ + \mathrm{e}^{\mathrm{i}\theta} a_-) \mathrm{e}^{-\mathrm{i}(n+1/2)\omega t} \mathrm{e}^{-\mathrm{i}kt} \mid \epsilon_{+,n}\rangle \\
&\qquad + \sqrt{\tfrac{1}{2}} (a_+ - \mathrm{e}^{\mathrm{i}\theta} a_-) \mathrm{e}^{-\mathrm{i}(n+1/2)\omega t} \mathrm{e}^{\mathrm{i}kt} \mid \epsilon_{-,n}\rangle\big) \\
&= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \mathrm{e}^{-\mathrm{i}(n+1/2)\omega t} \big((a_+ \cos kt - \mathrm{i}\mathrm{e}^{\mathrm{i}\theta} a_- \sin kt) \mid +, n\rangle \\
&\qquad + (\mathrm{e}^{\mathrm{i}\theta} a_- \cos kt - \mathrm{i} a_+ \sin kt) \mid -, n+1\rangle\big) \\
&= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \mathrm{e}^{-\mathrm{i}(n+1/2)\omega t} \big((a_+ \cos kt - \mathrm{i}\mathrm{e}^{\mathrm{i}\theta} a_- \sin kt) \mid +, n\rangle \\
&\qquad + (\mathrm{e}^{\mathrm{i}\theta} a_- \cos kt - \mathrm{i} a_+ \sin kt) \mathrm{e}^{\mathrm{i}\omega t} \mid -, n\rangle\big). \qquad (2.13)
\end{aligned}
$$

This gives the joint density operator

$$\rho_j(t) = \mid \Phi(t)\rangle\langle\Phi(t) \mid . \qquad (2.14)$$

This operator contains all of the information about both the electronic and photon evolutions. However we are only interested in the electronic degrees of freedom. To get rid of the redundant photon information, we trace out the photon degrees of freedom to give the electronic reduced density operator $\rho(t)$.

Now in general, we cannot expect a reduced density operator to describe a pure state. That is, we cannot expect that $\rho(t) = \mid \zeta(t)\rangle\langle\zeta(t) \mid$. This is because

the ignored degrees of freedom induce irreversibility into the system [Haake 1973]. However, for the semi-classical Jaynes-Cummings model we find that the reduced density operator is pure; the evolving state (2.13) can be written in the product form

$$\Phi(t) = \phi(t) \mid ze^{-i\omega t}\rangle, \tag{2.15}$$

where

$$\phi(t) = \begin{bmatrix} (a_+ \cos kt - ie^{i\theta} a_- \sin kt)e^{-i\omega t/2} \\ (e^{i\theta} a_- \cos kt - ia_+ \sin kt)e^{i\omega t/2} \end{bmatrix}. \tag{2.16}$$

Hence the reduced density operator has the form

$$\rho(t) = \mid \phi(t)\rangle\langle\phi(t) \mid . \tag{2.17}$$

Note that $\rho(t)$ does not determine $\phi(t)$ uniquely, as we are free to rephase ϕ arbitrarily. This point will be returned to later.

Now that we have the evolving electronic state, we want to find the electronic Hamiltonian that generates it. By direct substitution one can easily verify that the electronic dynamics is generated by the semi-classical Hamiltonian

$$H(t) = \begin{bmatrix} \frac{\omega}{2} & ke^{-i\omega t} \\ ke^{i\omega t} & -\frac{\omega}{2} \end{bmatrix}. \tag{2.18}$$

Note that H is time-dependent. Further, one can generate it from the time-dependent joint Hamiltonian H_j by naively replacing the boson creation operator b by the function $\exp\{i\omega t\}$.

As mentioned earlier in this section, the reduced density operator does not determine the phase of the evolving electronic state. Thus instead of $\phi(t)$, we could have taken

$$\zeta(t) = e^{-i\alpha(t)}\phi(t) \tag{2.19}$$

for any phase α. Then

$$\begin{aligned} i\dot{\zeta}(t) &= \dot{\alpha}e^{-i\alpha}\phi(t) + ie^{-i\alpha}\dot{\phi} \\ &= (H + \dot{\alpha})\zeta. \end{aligned} \tag{2.20}$$

Hence, taking $\zeta(t)$ instead of $\phi(t)$ merely leads to a time-dependent energy renormalisation.

Further, as I will show in section 3.1, this renormalisation does not affect the Berry phases. Hence we are free to take any normalisation we wish. The Hamiltonian form (2.18) is the most convenient for our purposes as it is traceless.

The semi-classical limit of the joint Hamiltonian (2.5) has also been found using other methods. For instance, Klenner *et al.* [1986] analyse the problem in Bargmann space. The problem is also treated rigorously by Raggio and Zivi [1985]. They use an asymptotic limit, taking $\lambda \to 0$ and $|z| \to \infty$ while holding $k = \lambda|z|$ constant. As these methods are mathematically complex and do not give any further physical insight into the origins of Hamiltonian time dependence, I will not discuss them any further.

Chapter Three

The Berry phase

In section 2.1 we saw that time-independent systems have stationary states. These are vectors that correspond to the same physical state throughout their evolution. In other words, at all times the evolving vectors return to their initial values up to a (dynamical) phase. In this chapter I will extend this result to the time-dependent case.

The natural extension of a time-independent Hamiltonian is a $\tilde{t}$-periodic one. That is, we take the Hamiltonian $H(t)$ to satisfy

$$H(t+\tilde{t}) = H(t) \tag{3.1}$$

for some $\tilde{t}$. In chapters 5 and 6, we will see that this property greatly facilitates the analysis of the problem. The non-periodic case is discussed in section 11.1.

Now a time-independent Hamiltonian is periodic with arbitrary period. Further, its eigenvectors return to themselves up to a phase at all times. This leads to the following definition in the $\tilde{t}$-periodic case. An initial state $\phi(0)$ is called a *cyclic initial state* of the $\tilde{t}$-periodic Hamiltonian H if

$$\phi(\tilde{t}) = \mathrm{e}^{\mathrm{i}\chi}\phi(0). \tag{3.2}$$

That is, the initial state need only return to itself up to a phase at time $\tilde{t}$. χ is called the *overall phase*. We will see that χ is not a simple generalisation of the dynamical phase of equation (2.3). This leads in the next section to the definition of Berry phase. Note that, in comparison to the adiabatic case, the cyclic initial states are not necessarily eigenvectors of the Hamiltonian.

A given Hamiltonian might not have any cyclic initial states. This problem also occurs for time-independent systems. There, the existence of stationary states depends on the existence of Hamiltonian eigenvectors, and these are not guaranteed to exist for systems with infinite-dimensional Hilbert spaces. This is discussed in chapter 8.

The rest of this chapter is organised as follows. In section 3.1 I discuss the nature of the overall phase χ. We find that it splits into the sum of two parts. The first is the time integral of the instantaneous expectation value of the Hamiltonian. As such, it is the natural generalisation of the dynamical phase present for time-independent systems. The remainder is called the Berry phase [Berry 1984]. In section 7.1, I will show that this phase is a geometric property of the evolution of the system in projective Hilbert space [Aharonov and Anandan 1987]. Finally, the Berry phase is then calculated using single-valued vectors.

Now two states which only differ by a phase are physically equivalent and so there is an arbitrary phase in quantum mechanics. This raises the question of the measurement of overall (and so Berry) phases. In section 3.2 I show that both of these phases can be measured by interference. There are two methods of doing this. In the first, two systems are prepared in identical initial states. They are then subjected to the action of different Hamiltonians. Their phase difference at some time $\tilde{t}$ can then be found by direct interference.

The second method of measuring phase differences is to start in a non-cyclic initial state. Then the phase differences of the cyclic components of the initial state can be measured by internal interference. This method is used in section 9.1, where I interpret the Rabi oscillations of quantum optics in terms of Berry phases [Moore 1990b, Tewari 1989]. Both of these approaches can be readily visualised by considering photon experiments [Chiao and Wu 1986]. Such systems are discussed at the end of section 3.2.

3.1 Definition

In the introduction to this chapter, I defined the cyclic initial states $\phi(0)$ of a $\tilde{t}$-periodic Hamiltonian $H(t)$. These are the initial states for which

$$\phi(\tilde{t}) = \mathrm{e}^{\mathrm{i}\chi}\phi(0). \tag{3.3}$$

In this section I investigate the nature of the overall phase χ.

At first sight, one might think that χ should be the natural generalisation of the dynamical phase:

$$\delta = -\int_0^{\tilde{t}} \langle \phi(t) \mid H(t) \mid \phi(t) \rangle \, \mathrm{d}t. \tag{3.4}$$

However this is not the case. There is an extra part γ called the *Berry phase*:

$$\gamma = \chi - \delta. \tag{3.5}$$

This was first discussed by Berry [1984] in the adiabatic context, with the generalisation to non-adiabatic evolution being provided by Aharonov and Anandan [1987].

To calculate the Berry phase, we use the notion of a single-valued vector [Moore and Stedman 1990c]. This is a vector $\psi(t)$ that follows the evolution of $\phi(t)$ up to a phase, and is single-valued in the sense that $\psi(\tilde{t}) = \psi(0)$. That is, a single-valued vector has the form

$$\psi(t) = \mathrm{e}^{-\mathrm{i}\theta(t)}\phi(t), \tag{3.6}$$

where $\theta(0) = 0$ and $\theta(\tilde{t}) = \chi$.

Note that there are an infinity of single-valued vectors for each evolving state. This is because we may choose the θ of equation (3.6) arbitrarily at all intermediate times. Further, one does not need to know $\phi(t)$ itself to find a single-valued vector. As we are choosing the phase of $\psi(t)$, we only need to know the path followed by the system in projective Hilbert space. Hence the fact that the Berry phases can

be calculated from the single-valued vectors (as shown by the following analysis) points to the geometric nature of the Berry phase. This is discussed in more detail in section 7.1.

I now turn to the calculation of Berry phases in terms of the single-valued vectors. As we are given the overall phase, all we need is the dynamical phase. By direct substitution into equation (3.4), we find that

$$\begin{aligned}\delta &= -\int_0^{\tilde{t}} \langle \phi(t) \mid H \mid \phi(t) \rangle \, \mathrm{d}t \\ &= -\mathrm{i} \int_0^{\tilde{t}} \langle \phi(t) \mid \dot{\phi}(t) \rangle \, \mathrm{d}t \\ &= \chi - \mathrm{i} \int_0^{\tilde{t}} \langle \psi(t) \mid \dot{\psi}(t) \rangle \, \mathrm{d}t. \end{aligned} \tag{3.7}$$

Hence, substituting into equation (3.5), we have that

$$\begin{aligned}\gamma &= \chi - \delta \\ &= \mathrm{i} \int_0^{\tilde{t}} \langle \psi(t) \mid \dot{\psi}(t) \rangle. \end{aligned} \tag{3.8}$$

Note that equation (3.8) has the same form as the adiabatic result of Berry. This connection is further explained in section 4.2. Equation (3.8) provides the starting point for the rest of the formalism in this thesis. In fact, I will show that the various methods used in the literature for calculating Berry phases merely provide a way of finding the single-valued vectors of the system. Hence single-valued vectors are an important unifying tool in the study of Berry phases.

For instance, Moore and Stedman [1990b] decompose the evolution operator into the product form

$$U(t) = Z(t)\mathrm{e}^{\mathrm{i}Mt}, \tag{3.9}$$

where Z is $\tilde{t}$-periodic. They find that the cyclic initial states $\phi_\alpha(0)$ are the eigenvectors of M and that the corresponding single-valued vectors can be taken to be

$$\psi_\alpha(t) = Z(t)\phi_\alpha(0). \tag{3.10}$$

This is discussed in more detail in section 5.1. Another example is provided by the Lie algebraic approach of section 7.2. There the single-valued vectors can be taken to be generalised coherent states.

Many simple results can be proved by the use of single-valued vectors. As already noted, the single-valued vectors only depend on the image of the evolution in projective Hilbert space. This points to the geometric nature of the Berry phase. Another example is the independence of the Berry phase on the energy normalisation. This was commented on in section 2.2 with reference to the semi-classical two-level atom.

Imagine that we know the evolution for some Hamiltonian $H(t)$. This gives the evolving cyclic initial state $\phi(t)$ and a corresponding single-valued vector $\psi(t)$. Renormalising the energy is achieved by replacing $H(t)$ by

$$H'(t) = E(t) + H(t) \tag{3.11}$$

for some scalar $E(t)$. Then it is easy to show that the energy renormalisation merely rephases the evolving state:

$$\phi'(t) = \exp\{-\mathrm{i}\int_0^t E(t')\,\mathrm{d}t'\}\phi(t). \tag{3.12}$$

Now the single-valued vectors follow the evolving state up to a phase. Hence we can use the same single-valued vectors for both Hamiltonians. This means that both Hamiltonians generate the same Berry phases. We note that, while the two states $\phi(\tilde{t})$ and $\phi'(\tilde{t})$ have the same Berry phases, they have different overall phases. In fact,

$$\chi' = \chi - \int_0^{\tilde{t}} E(t)\,\mathrm{d}t. \tag{3.13}$$

The difference manifests itself in the dynamical phase of the system. This fact is consistent with our identification of δ with the dynamical (energy dependent) part of the overall phase.

3.2 Measurement

In quantum mechanics, the physical states are the elements of the projective Hilbert space $\mathcal{P}$, not the vectors in the Hilbert space $\mathcal{H}$. In other words, the physical state corresponding to the vector ϕ is the density operator

$$\rho = |\,\phi\rangle\langle\phi\,|\,. \tag{3.14}$$

But the density operator is independent of the overall phase of the state ϕ. At first sight, this seems to imply that the overall phase (and so the Berry phase) is not measurable.

There are two related ways to avoid this problem. For the first, let H_1 and H_2 be two distinct Hamiltonians such that $\phi(0)$ is a cyclic initial state for both. Let $\phi(0)$ evolve into $\phi_1(t)$ under the action of H_1 and $\phi_2(t)$ under the action of H_2. Then, as $\phi(0)$ is a cyclic initial state, $\phi_1(\tilde{t}) = \exp\{i\chi_1\}\phi(0)$ and $\phi_2(\tilde{t}) = \exp\{i\chi_2\}\phi(0)$. The difference between their two overall phases can then be measured by interference.

A good example of this possibility is the intuitive explanation of the Aharonov-Bohm effect [Aharonov and Bohm 1959]. Here we imagine an electron beam diffracting both ways around a solenoid core. To a first approximation, this can be modelled by imagining that the initial electronic wavefunction evolves under each of two Hamiltonians (one for each side of the solenoid), the two resulting states being compared by interference at some later time.

The second method only involves one Hamiltonian H. Here we choose the initial state not to be cyclic. For example, we could take

$$\phi(0) = a_+\phi_+(0) + a_-\phi_-(0), \tag{3.15}$$

where the $\phi_\pm(0)$ are cyclic initial states. Then

$$\phi(\tilde{t}) = e^{i\chi_+}\phi_+(0) + e^{i\chi_-}\phi_-(0). \tag{3.16}$$

Assuming that $\chi_+ \neq \chi_-$, this is not equal to the initial state up to a phase. Hence the initial and final states are experimentally distinguishable. A similar analysis is undertaken by Datta [1989] in the context of quantum measurement theory.

Both of these methods measure the difference in overall phase of two cyclic initial states. This is because there is only one arbitrary phase in quantum mechanics. Hence, while $\exp\{i\chi\}\phi_1$ and ϕ_1 are physically equivalent, $\exp\{i\chi\}\phi_1 + \phi_2$ and $\phi_1 + \phi_2$ are not. In other words, we cannot independently rephase the components of the system's wavefunction. This means that the phase difference between the components of a wavefunction is measurable.

To make these measurement schemes more concrete, I will now discuss the Berry phases for photons. I follow Chiao and Wu [1986]. Consider a photon propagating down a helically wound optical fibre. The system has Hamiltonian

$$H = H_0 + \kappa \mathbf{s} \cdot \mathbf{k}, \tag{3.17}$$

where $\mathbf{k}$ is the direction of propagation and $\mathbf{s}$ is the spin operator. κ is a coupling constant and H_0 describes the background evolution. Note that the propagation direction follows the optical fibre.

The Hamiltonian H has eigenvectors $\mid \mathbf{k}, \sigma\rangle$, where $\sigma = \pm 1$ is the photon helicity. We have that

$$H_0 \mid \mathbf{k}, \sigma\rangle = E_0 \mid \mathbf{k}, \sigma\rangle, \tag{3.18}$$

$$\mathbf{s} \cdot \mathbf{k} \mid \mathbf{k}, \sigma\rangle = \sigma \mid \mathbf{k}, \sigma\rangle. \tag{3.19}$$

The coiling of the fibre is taken into account by varying $\mathbf{k}$; we can put $\mathbf{k} = \mathbf{k}(\ell)$, where ℓ is the optical path length. Further, assuming that the fibre does not have any sharp bends and we can ignore linear birefringence, the system maintains its helicity state. That is, the system is adiabatic. Hence if the initial state is given by

$$\mid \phi(0)\rangle = \mid \mathbf{k}(0), \sigma\rangle, \tag{3.20}$$

then the evolving state is given by

$$\mid \phi(\ell)\rangle = e^{i\theta_\sigma(\ell)} \mid \mathbf{k}(\ell), \sigma\rangle. \tag{3.21}$$

Now as the optical fibre is twisted into a helix, we have $\mathbf{k}(\tau) = \mathbf{k}(0)$ for some length τ. Hence from equation (3.21), the spin states are cyclic initial states with overall phases $\theta_\sigma(\tau)$. Further, we can take the vector $\mid \mathbf{k}(\ell), \sigma\rangle$ as our single-valued vector. From equation (3.8), this gives the Berry phase

$$\gamma_\sigma = \mathrm{i} \int_0^\tau \langle \mathbf{k}(\ell), \sigma \mid \tfrac{\mathrm{d}}{\mathrm{d}\ell} \mid \mathbf{k}(\ell), \sigma \rangle \, \mathrm{d}\ell. \tag{3.22}$$

Chiao and Wu [1986] show that this can be written in the form $\gamma = -\sigma\Omega$, where Ω is the solid angle subtended by $\mathbf{k}(\ell)$ at the origin. Note that if the helix is uniform, then $\mathbf{k}(\ell)$ follows a circle and so

$$\Omega = 2\pi N(1 - \cos\theta). \tag{3.23}$$

Here N is the winding number of the helix and θ is its pitch.

We are now in a position to illustrate the first measurement scheme discussed above. Imagine that we send identical beams down two counter-rotating fibres. Then it is a simple matter to prove that the two beams pick up opposite Berry phases and identical dynamical phases. Hence the interference intensity at the end of the fibres is directly related to the difference in Berry phases of the two beams.

To discuss the second approach, we need to start in a non-cyclic initial state. For example, we could start in a linearly polarised state:

$$\phi(0) = \sqrt{\tfrac{1}{2}} \mid \mathbf{k}(0), + \rangle + \sqrt{\tfrac{1}{2}} \mid \mathbf{k}(0), - \rangle. \tag{3.24}$$

Then as $\gamma_- = -\gamma_+$, the initial state $\phi(0)$ evolves into

$$\phi(\tau) = \sqrt{\tfrac{1}{2}} \mathrm{e}^{-\mathrm{i}(E_0\tau + \kappa\tau - \gamma_+)} \mid \mathbf{k}(0), + \rangle + \sqrt{\tfrac{1}{2}} \mathrm{e}^{-\mathrm{i}(E_0\tau - \kappa\tau + \gamma_+)} \mid \mathbf{k}(0), - \rangle. \tag{3.25}$$

Hence $|\langle \phi(0) \mid \phi(\tau) \rangle|^2 = \cos^2(\kappa\tau - \gamma_+)$. This means that, by Malus' theorem, the plane of polarisation of the light beam has rotated by the angle $\kappa\tau - \gamma_+$ [Chiao and Wu 1986]. Hence the Berry phases of the cyclic components of the initial state are directly measurable.

This result was experimentally verified by Tomita and Chiao [1986]. In fact, it was the first experiment designed specifically to test for the existence of Berry phases. Note that this result can also be explained classically. It can be interpreted in terms of the intrinsic topological structure of Maxwell's theory [Cai *et al.* 1990].

Chapter Four

The adiabatic case

In general, one must solve the time-dependent Schrödinger equation before one can find the Berry phases. However there are exceptions. For example, consider a Hamiltonian of the form $H(t) = \exp\{-\mathrm{i}At\}H(0)\exp\{\mathrm{i}At\}$, with A constant. As I will show in section 5.3, the single-valued vectors for this system can be written down directly from the Hamiltonian. Hence the corresponding Berry phases may be evaluated without having to first calculate the evolution operator.

In this chapter I will discuss another important set of simply solvable Hamiltonians. These are systems whose time dependence comes from the slow variation of some external parameters, such as the direction of an applied magnetic field. In this situation, one may use the adiabatic theorem to show that an eigenstate of the initial Hamiltonian $H(t)$ stays in a corresponding eigenstate of $H(t)$ [Avron *et al.* 1987]. The single-valued vectors are then just suitably rephased eigenvectors. This was the case considered by Berry [1984].

One of the most important applications of the adiabatic theorem is the Born-Oppenheimer approximation [Born and Oppenheimer 1927]. This is used to decouple the nuclear and electronic degrees of freedom of molecules. We find that a proper consideration of the effect of Berry phases leads to the presence of an effective vector potential [Moody *et al.* 1986]. In fact, this term was discussed by Mead and Truhlar [1979] before Berry phases were defined. Finally, a path integral treatment of the problem [Kuratsuji and Iida 1985] leads to the interpretation of field theoretic anomalies in terms of Berry phases [Semenoff 1986].

The rest of this chapter is organised as follows. In section 4.1 I state the adiabatic theorem. This is used to calculate the adiabatic Berry phases in section 4.2.

Finally, the application of Berry phases to the Born-Oppenheimer approximation is discussed in section 4.3.

4.1 The adiabatic theorem

The adiabatic theorem has long been a folk theorem in quantum mechanics. It states that if the surroundings of a system change slowly enough, then the evolution follows the eigenspaces of the time-dependent Hamiltonian. This result is very important as it provides the framework for, among other things, the Born-Oppenheimer approximation. In this section I give a proof of the adiabatic theorem first reported by Avron *et al.* [1987].

The following approach is used. We start with a time-dependent Hamiltonian $H(t)$, fixing our attention on a single spectral projection $P(t)$. This allows us to define a new Hamiltonian,

$$H_A(t,P) = H(t) + \mathrm{i}[\dot{P},P]. \tag{4.1}$$

This Hamiltonian will be referred to as the *adiabatic equivalent* of H. We find that an initial state in $P(0)$ evolves into a state in $P(t)$ under the action of H_A. The adiabatic theorem follows by noting that, in the adiabatic limit, the evolution operators corresponding to the two Hamiltonians coincide.

Before beginning the formal proof of the adiabatic theorem, I will explicitly construct the adiabatic equivalent of a simple Hamiltonian. Let $H(t)$ be the two-level Hamiltonian

$$H(t) = \begin{bmatrix} 0 & k\mathrm{e}^{-\mathrm{i}\omega t} \\ ke^{\mathrm{i}\omega t} & 0 \end{bmatrix}. \tag{4.2}$$

By direct substitution, one can easily show that this has eigenvectors

$$|\,\xi_{\pm}\rangle = \sqrt{\tfrac{1}{2}}\begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t} \\ \pm 1 \end{bmatrix}, \tag{4.3}$$

with eigenvales $E_{\pm} = \pm k$. Now, assume that $H_A(t,P_+)$ is known. Then

$$\begin{aligned} H_A(t,P_-) &= H(s) + \mathrm{i}\left(\tfrac{\mathrm{d}}{\mathrm{d}t}(1-P_+(t))(1-P_+(s)) - (1-P_+(s))\tfrac{\mathrm{d}}{\mathrm{d}t}(1-P_+(s))\right) \\ &= H(t) + \mathrm{i}(\dot{P}_+(s)P_+(s) - P_+(s)\dot{P}_+(s)) = H_A(t,P_+). \end{aligned} \tag{4.4}$$

Thus the adiabatic equivalent Hamiltonians for the two eigenspaces are the same. We have

$$\begin{aligned} P_+ &= |\,\xi_+\rangle\langle\xi_+\,| \\ &= \tfrac{1}{2}\begin{bmatrix} 1 & \mathrm{e}^{-\mathrm{i}\omega t} \\ \mathrm{e}^{\mathrm{i}\omega t} & 1 \end{bmatrix}. \end{aligned} \tag{4.5}$$

Hence

$$\mathrm{i}[\dot{P}_+, P_+] = \tfrac{\omega}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4.6}$$

Substituting into equation (4.1), the adiabatic equivalent Hamiltonian is then given by

$$\begin{aligned} H_A(t, P_+) &= H(t) + \mathrm{i}[\dot{P}_+, P_+] \\ &= \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix}, \end{aligned} \tag{4.7}$$

where the prime stands for differentiation with respect to time. This is just the Hamiltonian for the Jaynes-Cummings model with zero detuning.

I now turn back to the formal development. The proof of the adiabatic theorem is greatly facilitated by the introduction of the scaled time $s = t/T = \omega t$. Taking $T \to \infty$ corresponds to the adiabatic limit. We require that the Hamiltonian satisfies the following technical assumptions:

(i) H is self-adjoint, bounded from below and has a closed s-independent domain.

(ii) $H(s)$ is a k-times continuously differentiable function of s, where k will be specified later.

(iii) $H(s)$ has gaps in its spectrum and $P(s)$ is the spectral projection onto a finite band bordered by gaps.

These conditions are necessary to guarantee the existence and uniqueness of the evolution operators that will be introduced later.

As H is taken to be a function of s, so must the adiabatic equivalent of H:

$$H_A(s, P) = H(s) + \mathrm{i}\omega[P'(s), P], \tag{4.8}$$

where the prime stands for differentiation with respect to s.

We now introduce the evolution operators $U(s)$ and $U_A(s,P)$ corresponding to $H(s)$ and $H_A(s,P)$ respectively. These are the solutions of the time-dependent Schrödinger equations

$$\mathrm{i}\partial_s U(s) = TH(s)U(s), \tag{4.9}$$

$$\mathrm{i}\partial_s U_A(s,P) = TH_A(s,P)U_A(s,P) \tag{4.10}$$

that are equal to unity at $s = 0$. It turns out that for U to exist we require the constant k of condition (ii) to be at least two, while for U_A it must be at least three [Avron *et al.* 1987]. This is because the definition of H_A involves a derivative of P. Thus H_A has one order of differentiability less than H. Note that both evolution operators are unitary and strongly continuous in s.

We are now in a position to prove that the evolution under $H_A(s,P)$ follows the eigenspace $P(s)$ of $H(s)$. To do this, we must prove that $U_A(s,P)P(0) = P(s)U_A(s,P)$. In other words, we must show that $U_A(s,P)$ is an intertwining operator for $P(0)$ and $P(s)$ [Anderson and Camporesi 1990]. To do this we show that both sides satisfy the same initial value problem. This proof is taken from Avron *et al.* [1987] and is based on an idea of Kato [1950].

For $U_A(s,P)P(0)$ we have

$$\partial_s \left(U_A(s,P)P(0)\right) = -\mathrm{i}TH_A(s,P)\left(U_A(s,P)\right), \tag{4.11}$$

$$\left(U_A(s,P)P(0)\right)|_{s=0} = P(0). \tag{4.12}$$

The operator $P(s)U_A(s,P)$ obviously satisfies the same initial condition. Thus we merely need to check that it satisfies (4.6). The following lemma is required.

Lemma 4.1 *$P'(s) = P(s)P'(s) + P'(s)P(s)$ and $P(s)P'(s)P(s) = 0$.*

Proof: Both results follow from the fact the P is idempotent: $P^2 = P$. Differentiating with respect to s then gives the first result. But then

$$P(s)P'(s) = P'(s) - P'(s)P(s)$$

$$\Rightarrow \qquad P(s)P'(s)P(s) = P'(s)P(s) - P'(s)P^2(s)$$
$$= P'(s)P(s) - P'(s)P(s) = 0, \tag{4.13}$$

proving the second result. ∎

Thus, using the fact that $H(s)$ and $P(s)$ commute,

$$\begin{aligned}
\partial_s \left(P(s)U_A(s,P)\right) &= -\mathrm{i}TP(s)H_A(s,P)U_A(s,P) + P'(s)U_A(s,P) \\
&= -\mathrm{i}TP(s)\left(H(s) + \frac{\mathrm{i}}{T}[P'(s),P(s)]\right)U_A(s,P) \\
&\quad + \left(P(s)P'(s) + P'(s)P(s)\right)U_A(s,P) \\
&= -\mathrm{i}TH(s)P(s)U_A(s,P) + P'(s)P(s)U_A(s,P) \\
&= -\mathrm{i}T\left(H(s) + \frac{\mathrm{i}}{T}[P'(s),P(s)]\right)P(s)U_A(s,P) \\
&= -\mathrm{i}TH_A(s,P)\left(P(s)U_A(s,P)\right). \qquad (4.14)
\end{aligned}$$

We have seen that $U_A(s,P)P(0)$ and $P(s)U_A(s,P)$ satisfy the same inital value problem. Hence, as the solution of such an equation is unique, the two operators must be equal:

$$U_A(s,P)P(0) = P(s)U_A(s,P). \tag{4.15}$$

To recapitulate, we started with a given Hamiltonian $H(s)$. We then constructed another Hamiltonian $H_A(s,P)$ whose evolution follows a given eigenspace $P(s)$ of $H(s)$. Now $H_A(s,P)$ is formally a $1/T$ approximant to $H(t)$. Thus in the adiabatic limit ($T \to \infty$) the two Hamiltonians agree. Hence, we expect that the two evolution operators should also agree in the adiabatic limit. This gives us the adiabatic theorem.

To compare the two evolution operators $U(s)$ and $U_A(s,P)$, we need the wave operator

$$\Omega(s) = U_A^*(s,P)U(s). \tag{4.16}$$

The adiabatic theorem then follows by proving that $\Omega(s) \to 1$ as $T \to \infty$. This is done with the use of an iterative expansion.

Define the kernel

$$K(s,P) = U_A^*(s,P)[P'(s),P(s)]U_A(s,P), \tag{4.17}$$

and the operators

$$\Omega_0(s) = 1, \tag{4.18}$$

$$\Omega_j(s) = -\int_0^s K(s',P)\Omega_{j-1}(s')\,\mathrm{d}s'. \tag{4.19}$$

Then Avron *et al.*[1987] prove that

$$\Omega(s) - \sum_{j=0}^{N} \Omega_j(s) = \mathrm{O}(T^{-N}). \tag{4.20}$$

Hence Ω is just the sum of the Ω_j. Further, they show that

$$\sup\|\Omega_j(s)\| = \mathrm{O}(T^{1-j}) \qquad (j \geq 2). \tag{4.21}$$

Thus the terms Ω_j fall off as an inverse power of the adiabatic time scale T. A similar result has been reported by Nenciu and Rasche [1989].

These two results show that the wave operator tends to unity in the adiabatic limit. Thus the adiabatic limit of the evolution under $H(s)$ indeed follows the eigenspaces of $H(s)$. This proves the adiabatic theorem.

4.2 Berry phases

For most Hamiltonians, the time-dependent Schrödinger equation must be solved before the single-valued vectors, and so the Berry phases, can be found. However there are exceptions, perhaps the most important one being adiabatic Hamiltonians. As we will now see, for these systems the adiabatic theorem derived in the previous section allows us to write the single-valued vectors down directly from the Hamiltonian. In fact Berry phases were initially defined only for adiabatic Hamiltonians [Berry 1984, Holstein 1989]. The generalisation to arbitrary Hamiltonians was provided by Aharonov and Anandan [1987].

Let $H(\mathbf{R}(t))$ be a Hamiltonian whose only time dependence comes from the adiabatic variation of some parameters. For example, the system could be a spin in a slowly rotating magnetic field. Further, let $H(\mathbf{R}(t))$ have a one-dimensional eigenspace $\mathcal{M}(t)$ that does not cross any other levels. The case where $\mathcal{M}(t)$ is multi-dimensional is treated in section 11.1. Now take the parameter $\mathbf{R}$ around a closed curve with period $\tilde{t}$, so that the Hamiltonian is $\tilde{t}$-periodic. Then by the adiabatic theorem, an initial state $\phi(0)$ in $\mathcal{M}(0)$ evolves in such a way that the state at time t is in $\mathcal{M}(t)$. Now $\mathcal{M}(\tilde{t}) = \mathcal{M}(0)$ as $H(\tilde{t}) = H(0)$. Thus an initial state in $\mathcal{M}(0)$ returns to $\mathcal{M}(0)$. But as $\mathcal{M}(0)$ is one-dimensional, this means that the initial state $\phi(0)$ returns to itself up to a phase. In other words, the eigenvectors of the initial Hamiltonian $H(0)$ are cyclic initial states. Note that this does not hold for non-adiabatic Hamiltonians in general.

The adiabatic theorem does not tell us into which state in $\mathcal{M}(t)$ the initial state $\phi(0)$ evolves. However for calculating the Berry phases, all we need is a single-valued vector that follows the evolving state up to a phase. Hence, as the elements of $\mathcal{M}(t)$ are all equal up to a phase, we need merely choose a single-valued element of $\mathcal{M}(t)$. In other words, we need a single-valued eigenvector $\psi(\mathbf{R}(t))$ of $H(\mathbf{R}(t))$. Substituting into equation (3.8) then gives

$$\gamma = \mathrm{i} \int_0^{\tilde{t}} \langle \psi(\mathbf{R}(t)) \mid \dot{\psi}(\mathbf{R}(t)) \rangle \, \mathrm{d}t. \tag{4.22}$$

Further, as the time dependence of ψ is solely due to the variation of the parameters, we have $\dot{\psi}(\mathbf{R}(t)) = \nabla_{\mathbf{R}}\psi(\mathbf{R}) \cdot \dot{\mathbf{R}}(t)$. Thus we obtain Berry's result [Berry 1984]

$$\gamma = \mathrm{i} \oint \mathbf{A} \cdot \mathrm{d}\mathbf{R}, \tag{4.23}$$

where the one-form $\mathbf{A}$ is given by

$$\mathbf{A} = \langle \psi(\mathbf{R}) \mid \nabla_{\mathbf{R}}\psi(\mathbf{R}) \rangle. \tag{4.24}$$

This can also be written as a surface integral by the use of Stokes theorem;

$$\gamma = -\int\int \mathbf{F} \cdot \mathrm{d}\mathbf{S}. \tag{4.25}$$

Note that the one-form $\mathbf{A}$ and the two-form $\mathbf{F}$ can be interpreted as a gauge potential and field respectively.

This formalism can be extended to take account of the finite velocity with which the parameters move in any real system. In this case we find that the amplitude of a transition from one energy level to another also contains a geometrical part [Berry 1990a]. This has been verified by experiment [Zwanziger, Rucker and Chingas 1990]. Note that the geometric nature of the transition probabilities persists in the non-adiabatic regime [Anandan and Aharonov 1990]. This is discussed in more detail in section 11.1.

It is instructive to discuss the differences between the adiabatic and non-adiabatic definitions as given by Berry [1984] and Aharonov and Anandan [1987]. Berry only needs the adiabatic theorem because of his choice of initial states. Taking these to be the instantaneous eigenvectors of $H(0)$ means that the adiabatic approximation is necessary to ensure that the initial states are indeed cyclic. This is discussed by Moore and Stedman [1990b].

A good example of the adiabatic formalism is a spin in a slowly rotating magnetic field

$$H = \mu \mathbf{n} \cdot \boldsymbol{\sigma}. \tag{4.26}$$

The parameters are the direction of the magnetic field,

$$\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{4.27}$$

There is a subtlety here. For $\mathbf{n} = (0, 0, \pm 1)$, the angle ϕ is not well defined. It can be shown that the sphere S^2 does not have a globally well-defined smooth coordinate system. That is, as a differentiable manifold its atlas must contain at least two charts [Schutz 1988, p26]. This fact is of crucial importance in allowing the system to have non-trivial Berry phases [Liang 1989].

To calculate the Berry phases we need the eigenvectors of the Hamiltonian. By direct substitution, one may easily verify that the eigenvector of the eigenvalue μ can be written in either of the two forms [Stone 1986]

$$\zeta_+^{(1)} = \begin{bmatrix} \cos\frac{\theta}{2} \\ \mathrm{e}^{\mathrm{i}\phi}\sin\frac{\theta}{2} \end{bmatrix}, \tag{4.28}$$

$$\zeta_+^{(2)} = \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix}. \tag{4.29}$$

We need the two forms because ϕ is not defined at $\mathbf{n} = (0, 0, 1)$. At $\theta = 0$, the vector $\zeta_+^{(1)}$ is well-defined, whereas $\zeta_+^{(2)}$ is well-defined at $\theta = \pi$.

Now neither of these eigenvectors is single-valued; as $\sin(\theta + \pi) = -\sin\theta$ and $\cos(\theta + \pi) = -\cos\theta$, they both come back to their negatives. Thus the corresponding single-valued vectors $\psi_+^{(1)}$ and $\psi_+^{(2)}$ are found by multiplying by some phase α with $\alpha(0) = 0$ and $\alpha(\tilde{t}) = \pi$. The one-forms $\mathbf{A}_+^{(1)}$ and $\mathbf{A}_+^{(2)}$ and two-form $\mathbf{F}$ can then be shown to be the gauge potential and field of a magnetic monopole of strength $-1/2$ [Berry 1984]. Further, the Berry phase is just half of the solid angle that $\mathbf{n}(t)$ subtends at the origin. This result can easily be extended to any spin.

The adiabatic theorem is not only useful calculationally, it also allows us to derive many important general results. Here I will discuss the effect that time-reversal invariance has on the adiabatic Berry phase. The arguments given here are taken from Kivelson and Rokhsar [1988]. These results are based on the fact that the eigenvectors of a time-reversal invariant Hamiltonian can be chosen to be

real [Messiah 1964, p675]. However, this does not necessarily mean that we can choose the single-valued vectors $\psi(\mathbf{R})$ to be real, as this particular phase choice might not be single-valued. Of course, the single-valued vectors can be written as

$$\psi(\mathbf{R}(t)) = \mathrm{e}^{-\mathrm{i}\theta(t)}\zeta(\mathbf{R}(t)), \tag{4.30}$$

where $\zeta(\mathbf{R})$ is real.

We take $\psi(\mathbf{R}(0)) = \zeta(\mathbf{R}(0))$. Now $\zeta(\mathbf{R}(\tilde{t}))$ must equal $\zeta(\mathbf{R}(0))$ up to a phase as $\mathcal{M}(\tilde{t}) = \mathcal{M}(0)$. However, both vectors are real. Thus $\zeta(\mathbf{R}(\tilde{t})) = \pm\zeta(\mathbf{R}(0))$. As $\psi(\mathbf{R}(\tilde{t})) = \psi(\mathbf{R}(0))$ by hypothesis, this means that

$$\theta(\tilde{t}) = n\pi \tag{4.31}$$

for some integer n. Hence to calculate the Berry phases, all we need is the inner product $\langle\zeta(\mathbf{R}(t)) \mid \dot{\zeta}(\mathbf{R}(t))\rangle$. But as $\zeta(\mathbf{R}(t))$ is normalised and real, we have

$$\begin{aligned} & 1 = \int \zeta^2(\mathbf{R}(t))\,\mathrm{d}\mathbf{x} \\ \Rightarrow \qquad & 0 = \tfrac{\mathrm{d}}{\mathrm{d}t}\int \zeta^2(\mathbf{R}(t))\,\mathrm{d}\mathbf{x} \\ & \quad = \int \zeta(\mathbf{R}(t))\dot{\zeta}(\mathbf{R}(t))\,\mathrm{d}\mathbf{x} \\ & \quad = \langle\zeta(\mathbf{R}(t)) \mid \dot{\zeta}(\mathbf{R}(t))\rangle. \end{aligned} \tag{4.32}$$

Thus the Berry phases are given by

$$\begin{aligned} \gamma &= \mathrm{i}\int_0^{\tilde{t}} \langle\psi(\mathbf{R}(t)) \mid \dot{\psi}(\mathbf{R}(t))\rangle\,\mathrm{d}t \\ &= \mathrm{i}\int(-\mathrm{i}\dot{\theta})\,\mathrm{d}t \\ &= n\pi. \end{aligned} \tag{4.33}$$

To recapitulate, time-reversal invariance forces the Berry phases to be multiples of π. That is it forces them to be real in the sense that $\exp\{\mathrm{i}\pi\} = \pm 1$. Time-reversal invariant Fermi systems have been discussed by Avron *et al.* [1988]. I now give an example of a non-time-reversal invariant system, showing how it can lead to a complex Berry phase [Moore and Stedman 1990a].

Consider a five atom molecule with the following symmetry. Four identical ions are placed at the corners of a square with a single Jahn-Teller active ion at the square's centre [Stedman 1983]. Then the molecule has D_4 symmetry. When the ligand ions are held at these positions, the p_x and p_y orbitals of the central ion are degenerate. However, by the Jahn-Teller theorem [Sturge 1967], the molecule must have at least one vibrational mode that breaks this degeneracy. Our example has two, the B_1 and B_2 modes. Another mode of interest is the A_2 mode. This is just a joint rotation of the ligands about the central ion.

For convenience, we require that the couplings of the central ion to the two Jahn-Teller modes be equal. This gives the Jahn-Teller problem an extra $SO(2)$ symmetry. Including coupling to the A_2 mode, the second quantised Hamiltonian is then [Moore and Stedman 1990a]

$$\begin{aligned} H = {} & E(f_1^* f_1 + f_2^* f_2) + \omega_a(a^* a + \tfrac{1}{2}) + \omega_b(b_1^* b_1 + b_2^* b_2 + 1) \\ & + V_b\left((f_1^* f_1 - f_2^* f_2)(b_1 + b_1^*) + (f_1^* f_2 + f_2^* f_1)(b_2 + b_2^*)\right) \\ & + V_a(f_1^* f_2 - f_2^* f_1)(a - a^*). \end{aligned} \tag{4.34}$$

Here a^* creates a phonon in the A_2 mode, b_1^*, b_2^* create phonons in the two B modes and f_1^*, f_2^* create electrons in the p_x and p_y states.

Note that the coupling of the two B modes to the ion involves the "position" operators $Q_i = b_i + b_i^*$ and is therefore time-even. However, the A_2 coupling involves the "momentum" operator $P_a = a - a^*$ and so is time-odd. We will see that it is this term that permits the Berry phases to be complex.

To do this, we rewrite the Hamiltonian (4.34) in terms of the spin operators of the fermion doublet. This allows us to cast the problem into the form (4.26). It turns out to be convenient to work in the basis transformed by the operator

$$V = \sqrt{\tfrac{1}{2}} \begin{bmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{bmatrix} \tag{4.35}$$

Then it is easily shown that [Moore and Stedman 1990a]

$$H = E1 + \mathbf{B} \cdot \boldsymbol{\sigma}, \tag{4.36}$$

where $\mathbf{B} = (V_b Q_1, V_b Q_2, -V_a P_a)$ is an effective operator magnetic field. We ignore the $E1$ term as it only generates an extra dynamical phase. Thus the Hamiltonian is manifestly of the form (4.26).

First let us consider the time-even case. This corresponds to restricting $\mathbf{B}$ to the xy plane. Then the cone drawn by the spin during an adiabatic evolution is a plane, thereby subtending the solid angle 2π. Hence the time-reversal even Berry phase is π. However once the time-odd coupling is introduced, the cone subtends a smaller angle. Thus the Berry phase can be complex in general. Other effects of time-odd coupling in physics are discussed in appendix C.

Adiabatic Berry phases in the Jahn-Teller problem have also been discussed for other systems. For example, Chancey and O'Brien [1988] discuss the octahedral $T_1 \otimes (\epsilon_g \oplus \tau_{2g})$ case. Further, Ham [1987] shows that the level ordering of the lowest lying vibronic states in the $E \otimes \epsilon$ Jahn-Teller system is a good test for the existence of Berry phases. If Berry phases exist then the lowest state must have E symmetry, while if Berry phases do not exist then the symmetry must be A_1. As E symmetry is observed, the existence of Berry phases is verified. Observable consequences of the Berry phase for this system are also discussed by Zwanziger and Grant [1987].

4.3 The Born-Oppenheimer approximation

A major application of the adiabatic Berry phase is the Born-Oppenheimer approximation. We find that the usual result is incomplete due to the neglect of Berry phase terms. This was first noted by Mead and Truhlar [1979]. This result is not only important in quantum mechanics as it can also be used to explain field theoretic anomalies [Semenoff 1986].

This discussion will be structured as follows. First the effect of the Berry phase on the Born-Oppenheimer approximation is analysed following Moody *et al.* [1986]. To derive the corresponding field theoretic result, the quantum mechanical case is recast in the path integral approach [Kuratsuji and Iida 1985]. The generalisation to field theory is then straightforward [Semenoff 1986].

We start with the quantum mechanical Born-Oppenheimer approximation [Born and Oppenheimer 1927]. Imagine a molecular Hamiltonian

$$H(R,r) = -\frac{1}{2m_N}\nabla_R^2 + h(R,r), \tag{4.37}$$

where R represents the nuclear degrees of freedom and r the electronic ones. The operator $h(R,r)$ contains the electronic potential and kinetic energies and the coupling between the nuclear and electronic variables.

Our task is to find the vibronic eigenstates. To do this we assume that the nuclear motion is far slower than the electronic motion, allowing us to treat the electronic part of the problem quasi-statically. Thus we introduce the electronic eigenstates $\mid n(R)\rangle$:

$$h(R,r) \mid n(R)\rangle = \epsilon_n(R) \mid n(R)\rangle. \tag{4.38}$$

Note that $h(R,r)$ can be treated as an electronic Hamiltonian parameterised by the nuclear coordinates R. Thus we can calculate the adiabatic Berry phase that arises when we take R through a closed path. These Berry phases are just the line integrals of the one-forms

$$\mathrm{A}_n = \mathrm{i}\langle n(R) \mid \nabla_R \mid n(R)\rangle. \tag{4.39}$$

We will see that these effective vector potentials also appear in the effective Born-Oppenheimer Hamiltonian for the nuclear degrees of freedom.

The Born-Oppenheimer approximation essentially assumes that we can ignore the transition terms $\langle m(R) \mid \nabla_R \mid n(R)\rangle$ for $n \neq m$, although more refined formulations are available [Witkowski 1990]. This means that the Hamiltonian (4.37) has eigenvectors

$$\Psi_n = \Phi_n(R) \mid n(R)\rangle. \tag{4.40}$$

To find $\Phi_n(R)$ we must diagonalise the effective nuclear Hamiltonian $H_n(R) = \langle n(R) \mid H(R,r) \mid n(R,r)\rangle$. Let Ξ and Ξ' be arbitrary nuclear functions. Then

$$\begin{aligned} \nabla_R^2(\Xi \mid n\rangle) &= (\nabla_R^2\Xi) \mid n\rangle + 2(\nabla_R\Xi)\cdot(\nabla_R \mid n\rangle) \\ &\quad + \Xi(\nabla_R^2 \mid n\rangle) \\ \Rightarrow \qquad \langle n\Xi' \mid \nabla_R^2 \mid \Xi n\rangle &= \langle \Xi' \mid \nabla_R^2 \mid \Xi\rangle - 2\mathrm{i}\langle \Xi' \mid \nabla_R \mid \Xi\rangle \cdot \mathbf{A}_n \\ &\quad - \langle \Xi' \mid \Xi\rangle \mathbf{A}_n^2, \end{aligned} \tag{4.41}$$

where $\mathbf{A}_n$ is defined by equation (4.39).

Hence the Born-Oppenheimer Hamiltonian has the form

$$H_n = -\frac{1}{2m_N}(\nabla_R - \mathrm{i}\mathbf{A}_n)^2 + \epsilon_n(R). \tag{4.42}$$

Thus the electronic degrees of freedom have two effects on the nuclear motion. The first is the well-known modification of the potential energy term $\epsilon_n(R)$. The second is the presence of an effective vector potential $\mathbf{A}_n$. Most treatments assume that the electronic eigenvectors $\mid n(R)\rangle$ can be chosen to be real so that $\mathbf{A}_n$ vanishes [Merzbacher 1970, p77]. However Mead and Truhlar [1979] showed that, in general, this could not be achieved with a differentiable choice of phase.

The above analysis has shown that the effective Born-Oppenheimer Hamiltonian for the nuclear degrees of freedom contains a vector potential term. Further, this vector potential is just the generator of the electronic adiabatic Berry phases [Mead 1987]. These terms also appear in slow atomic collisions [Zygelman 1987].

It is instructive to recast this result in the path integral approach [Kuratsuji and Iida 1985]. We are interested in the diagonal matrix elements

$$\langle n(R_0)R_0 \mid \exp\{-\mathrm{i}HT\} \mid n(R_0)R_0\rangle \tag{4.43}$$

for some time T. After some formal manipulation, we find that

$$\langle n(R_0)R_0 \mid \exp\{-\mathrm{i}HT\} \mid n(R_0)R_0\rangle = \oint \mathcal{D}R\mathcal{D}P\exp\{\mathrm{i}(S_n + \gamma_n(C))\}, \tag{4.44}$$

where we integrate over all closed paths starting at R_0 and taking time T. The adiabatic action is given by $S_n = S_0 - \int_0^T \epsilon_n(t)\,\mathrm{d}t$, where $\epsilon_n(t)$ is the instantaneous energy.

We can see the effective nuclear action contains a term due to the Berry phase. Hence Berry phases have a manifest effect on the Born-Oppenheimer approximation in both the Hamiltonian (equation 4.42) and path integral (equation 4.44) approaches. A similar result is obtained by Düsedau [1988] for a spin-$\frac{1}{2}$ system in an external magnetic field.

This result leads to the connection between Berry phases and anomalies [Semenoff 1986]. Consider a system of interacting fermions and gauge fields. To a good approximation, we can treat the gauge fields as merely providing an effective potential in which the fermions move. In other words, we can treat the problem in the Born-Oppenheimer approximation, the fermions being the fast system and the gauge fields the slow system. Thus, by the argument presented above, the effective gauge field action will contain a vector potential term due to the smeared fermionic motion.

Now for some systems, such as the chiral Schwinger model, this extra vector potential destroys the gauge invariance of the action. Further, this gauge variance cannot be cancelled by the addition of counterterms. In other words, the theory is anomalous. The presence of anomalies in gauge field actions is highly undesirable, since they lead to such problems as a loss of unitarity or renormalisability [Collins 1989, pp331-353]. This problem has also been treated in the Hamiltonian context by Nelson and Alvarez-Guamé [1985].

The Born-Oppenheimer theory presented above has also been applied to quantum gravity [Brout and Venturi 1989]. Here matter is taken to follow gravity adiabatically, as the particle masses involved are much smaller than the Planck mass [Balbinot *et al.* 1990].

Chapter Five

Operator formalisms

Having discussed adiabatic Hamiltonians, I now return to the general case. As discussed in section 3.1, given the cyclic initial states $\phi_\alpha(0)$, the Berry phases can be calculated using the corresponding single-valued vectors. To use this algorithm one must first solve the time-dependent Schrödinger equation for an arbitrary initial state. Then one can find the cyclic initial states and, by rephasing the evolving state $\phi_\alpha(t)$, the single-valued vectors. However, this is a somewhat ad hoc approach.

In this chapter I formalise the process by decomposing the evolution operator U into the product form

$$U(t) = \mathbf{U}(t)\mathbf{R}(t) \tag{5.1}$$

in such a way that the operator $\mathbf{R}$ gives the cyclic initial states and the operator $\mathbf{U}$ generates the corresponding single-valued vectors. As mentioned in section 3.1, to each evolution there correspond many single-valued vectors. The operator decomposition schemes discussed below merely pick a convenient one of these for each cyclic initial state.

The rest of this chapter is organised as follows. In section 5.1 the decomposition scheme of Moore and Stedman [1990b] is discussed. As well as being computationally convenient for many problems, this formalism is very useful as the starting point for further investigations. For example, it allows a partial identification of those systems which have a complete set of cyclic initial states. This will be analysed in chapter 8. Further, it gives the basis for the Fourier theory of

the next chapter. This allows the cyclic initial states and Berry phases to be calculated directly from the Fourier components of the Hamiltonian, without having to evaluate the evolution operator first.

In section 5.2 the concept of quasi-degeneracy is discussed. Two cyclic initial states are said to be quasi-degenerate if they have the same overall phase. This property can be used to clarify the relationship between Berry phases and the time dependence of the Hamiltonian, as discussed in Moore [1990b].

In section 5.3 the decomposition of Salzman [1974] is given. This decomposition holds for a special class of Hamiltonians, including the cranked Hamiltonians of Wang [1990a, 1990b]. For these systems we can find the operators $\mathbf{U}$ and $\mathbf{R}$ without having to first calculate the evolution operator U. Finally, in section 5.4, we discuss a modification of the scheme of Cheng and Fung [1989]. This scheme is very general, including both of the earlier ones. However its very generality makes it hard to apply, as the cyclic initial states must be calculated from the evolution operator before $\mathbf{U}$ and $\mathbf{R}$ can be evaluated.

5.1 Moore and Stedman's decomposition

In this section I will describe the operator decomposition scheme of Moore and Stedman [1990b]. This scheme uses a decomposition that is a simple generalisation to all Hilbert spaces of the work done by Floquet [1883] on systems of linear differential equations with periodic coefficients. For a good summary of Floquet's results see Cronin [1980, pp95-106].

As mentioned earlier, the operator decomposition schemes are all ways of picking a convenient single-valued vector ψ from the relevant equivalence class $[\psi]$. Moore and Stedman's decomposition is chosen to pick the simplest representative from each class. Let the cyclic initial state $\phi(0)$ evolve into $\phi(t)$ under the action of a $\tilde{t}$-periodic Hamiltonian $H(t)$. Further let $\phi(0)$ have overall phase χ so that

$$\phi(\tilde{t}) = \mathrm{e}^{\mathrm{i}\chi}\phi(0). \tag{5.2}$$

Then all of the single-valued vectors corresponding to $\phi(t)$ have the form

$$\psi(t) = \mathrm{e}^{\mathrm{i}\theta(t)}\phi(t) \tag{5.3}$$

for some phase $\theta(t)$ with $\theta(\tilde{t}) = -\chi$. The simplest such phase is just

$$\theta(t) = -\chi t/\tilde{t}. \tag{5.4}$$

To find the evolution operator decomposition corresponding to this phase we need the following definition: a time-dependent operator F is a *unitary fundamental operator* of the Hamiltonian H iff F is unitary and $\mathrm{i}\dot{F} = HF$. An obvious example is the evolution operator U. Now let H be $\tilde{t}$-periodic and $X(t) \equiv F^*(t)F(t+\tilde{t})$. As F is a unitary fundamental operator of H, $\mathrm{i}\dot{F} = HF$. In particular we can substitute $t + \tilde{t}$ for t, so that

$$\begin{aligned} \mathrm{i}\dot{F}(t+\tilde{t}) &= H(t+\tilde{t})F(t+\tilde{t}) \\ &= H(t)F(t+\tilde{t}). \end{aligned} \tag{5.5}$$

Further, as $F(t+\tilde{t}) = F(t)X(t)$, we can use the chain rule to give

$$\begin{aligned} \mathrm{i}\dot{F}(t+\tilde{t}) &= \mathrm{i}\dot{F}(t)X(t) + \mathrm{i}F(t)\dot{X}(t) \\ &= H(t)F(t)X(t) + \mathrm{i}F(t)\dot{X}(t) \\ &= H(t)F(t+\tilde{t}) + \mathrm{i}F(t)\dot{X}(t). \end{aligned} \tag{5.6}$$

Comparing these two results we can see that $\mathrm{i}F(t)\dot{X}(t) = 0$. However, F is invertible so that $\dot{X} = 0$ and X is constant. To summarise, for every unitary fundamental operator of a $\tilde{t}$-periodic Hamiltonian, there exists a constant operator X such that $F(t+\tilde{t}) = F(t)X$. For the evolution operator U, the operator X is simply the monodromy operator $U(\tilde{t})$. The monodromy operator derives its name from the fact that it generates the long term evolution of the system: $U(n\tilde{t}+t) = U(\tilde{t})^n U(t)$ [Pressley and Segal 1986, p.124].

This result can be used to derive an evolution operator decomposition as follows. Let F be a unitary fundamental operator for the $\tilde{t}$-periodic Hamiltonian H such that $F(t+\tilde{t}) = F(t)X$. Note that X is unitary. In section A.1 I show that for every unitary operator X there exists a unique self-adjoint operator Y, with spectrum in the half-open interval $[0, 2\pi)$, such that $X = \exp\{\mathrm{i}Y\}$. Let $Q = Y/\tilde{t}$ and $P = F\exp\{-\mathrm{i}Qt\}$. Then $F = P\mathrm{e}^{\mathrm{i}Qt}$. Further

$$\begin{aligned} P(t+\tilde{t}) &= F(t+\tilde{t})\mathrm{e}^{-\mathrm{i}Q(t+\tilde{t})} \\ &= F(t)\mathrm{e}^{\mathrm{i}Q\tilde{t}}\mathrm{e}^{-\mathrm{i}Q(t+\tilde{t})} \\ &= F(t)\mathrm{e}^{-\mathrm{i}Qt} = P(t). \end{aligned} \tag{5.7}$$

Thus we have proved the following result:

Theorem 5.1 *Let F be a fundamental operator of the $\tilde{t}$-periodic Hamiltonian H. Then there exist unique operators P and Q with $F = P\exp\{\mathrm{i}Qt\}$, such that P is unitary and $\tilde{t}$-periodic and $Q\tilde{t}$ is self-adjoint and constant with spectrum in $[0, 2\pi)$.*

The condition on the spectrum of $Q\tilde{t}$ will be relaxed in the next section when I discuss quasi-degeneracy.

Decompositions of this type have attracted much interest in the study of periodic systems [Barone *et al.*1977, Maricq 1986, Salzman 1974]. When applied to the evolution operator, theorem 5.1 is the decomposition of Moore and Stedman, where the operators **U** and **R** of equation (5.1) are given by P and $\exp\{\mathrm{i}Qt\}$ respectively. To distinguish this case from the others, I will write the decomposition as

$$U = Z\mathrm{e}^{\mathrm{i}Mt}. \tag{5.8}$$

As $U(0) = 1$ we can see that $Z(0)$ is also unity. Z and M are simply related. Upon substituting equation (5.8) into the time-dependent Schrödinger equation $\mathrm{i}\dot{U} = HU$, we find that $HZ = \mathrm{i}\dot{Z} - ZM$. Substituting $t = 0$ then gives

$$M = -H(0) + \mathrm{i}\dot{Z}(0). \tag{5.9}$$

I will now show how the cyclic initial states and Berry phases can be recovered from the decomposition (5.8). Consider an arbitrary initial state $\phi(0)$ that evolves into $\phi(t) = U(t)\phi(0)$. Then $\phi(0)$ is a cyclic initial state with overall phase χ iff $U(\tilde{t})\phi(0) = \exp\{\mathrm{i}\chi\}\phi(0)$. Thus the cyclic initial states are precisely the eigenvectors of the monodromy operator $U(\tilde{t})$. However, as $Z(0) = 1$ and Z is $\tilde{t}$-periodic, we have that $Z(\tilde{t}) = 1$ and so $U(\tilde{t}) = \exp\{\mathrm{i}M\tilde{t}\}$. Thus, as the eigenvectors of $U(\tilde{t})$ and M coincide, the cyclic initial states are precisely the eigenvectors of M. Further, the overall phases are just the corresponding eigenvalues of $M\tilde{t}$. Hence the cyclic initial states can be found from M. Note that there can only be a complete set of cyclic initial states if M is diagonalisable, that is if M has a complete set of eigenvectors.

Now that we have the cyclic initial states $\phi_\alpha(0)$ and their overall phases χ_α, we need to calculate the corresponding Berry phases. To do this we must find a single-valued vector for each cyclic initial state. We try $\psi_\alpha(t) = Z(t)\phi_\alpha(0)$. Obviously $\psi_\alpha(t)$ is single-valued, so that we need merely show that it follows the evolving state $\phi_\alpha(t)$ up to a phase. We have that

$$\phi_\alpha(t) = Z(t)\mathrm{e}^{\mathrm{i}Mt}\phi_\alpha(0)$$

$$
\begin{aligned}
&= \mathrm{e}^{\mathrm{i}\chi_\alpha t/\tilde{t}} Z(t)\phi_\alpha(0) \\
&= \mathrm{e}^{\mathrm{i}\chi_\alpha t/\tilde{t}} \psi_\alpha(t).
\end{aligned} \tag{5.10}
$$

Hence we can evaluate the relevant single-valued vectors from the operator Z and the cyclic initial states. Note that this choice of single-valued vector does indeed have the simplest phase (5.4). To find the Berry phase of the cyclic initial state $\phi_\alpha(0)$ we need merely apply equation (3.8) to give

$$
\begin{aligned}
\gamma &= \mathrm{i}\int_0^{\tilde{t}} \langle \psi_\alpha(t) \mid \dot{\psi}_\alpha(t) \rangle \, \mathrm{d}t \\
&= \mathrm{i}\int_0^{\tilde{t}} \langle \phi_\alpha(0) \mid Z^*(t)\dot{Z}(t) \mid \phi_\alpha(0) \rangle \, \mathrm{d}t,
\end{aligned} \tag{5.11}
$$

the result given by Moore and Stedman [1990b].

Given any other single-valued vector ψ'_α corresponding to the cyclic initial state $\phi_\alpha(0)$, the vector ψ_α can be recovered from equation (5.3). We have just shown that $\phi_\alpha(t) = \exp\{\mathrm{i}\chi_\alpha t/\tilde{t}\}\psi_\alpha(t)$. To connect ψ'_α with ψ_α we must find the equivalent relation for ψ'_α. Writing $\psi'_\alpha(t) = \exp\{-\mathrm{i}\theta(t)\}\phi_\alpha(t)$, where $\theta(0) = 0$, we have

$$
\begin{aligned}
& \mathrm{i}\dot{\phi}_\alpha = H\phi_\alpha \\
\Rightarrow \quad & \mathrm{i}\dot{\psi}'_\alpha - \dot{\theta}\psi'_\alpha = H\psi'_\alpha \\
\Rightarrow \quad & \dot{\theta} = \mathrm{i}\langle \psi'_\alpha \mid \dot{\psi}'_\alpha \rangle - \langle \psi'_\alpha \mid H \mid \psi'_\alpha \rangle \\
\Rightarrow \quad & \theta = \mathrm{i}\int_0^t \langle \psi'_\alpha \mid \dot{\psi}'_\alpha \rangle \, \mathrm{d}t - \int_0^t \langle \psi'_\alpha \mid H \mid \psi'_\alpha \rangle \, \mathrm{d}t.
\end{aligned} \tag{5.12}
$$

Thus ψ_α and ψ'_α are connected by

$$
\psi_\alpha(t) = \mathrm{e}^{\mathrm{i}\left(\theta(t) - \chi_\alpha t/\tilde{t}\right)} \psi'_\alpha. \tag{5.13}
$$

As an example of the calculational utility of this decomposition, consider the semi-classical Jaynes-Cummings model with zero detuning. From equation (2.18), the Hamiltonian is given by

$$
H = \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix}, \tag{5.14}
$$

where $\omega = 2\pi/\tilde{t}$. We try

$$Z = \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t} & 0 \\ 0 & 1 \end{bmatrix}, \tag{5.15}$$

$$M = \begin{bmatrix} \frac{\omega}{2} & -k \\ -k & \frac{\omega}{2} \end{bmatrix}. \tag{5.16}$$

As Z is $\tilde{t}$-periodic and unitary and M is constant and self-adjoint, we need merely show that $U = Z\exp\{\mathrm{i}M\tilde{t}\}$ satisfies the Schrödinger equation. By direct computation we have

$$\begin{aligned} \mathrm{i}\dot{U} &= \left(\mathrm{i}\dot{Z} - ZM\right)\mathrm{e}^{\mathrm{i}Mt} \\ &= \begin{bmatrix} \frac{\omega}{2}\mathrm{e}^{-\mathrm{i}\omega t} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k & \frac{\omega}{2} \end{bmatrix} \\ &= HZ\mathrm{e}^{\mathrm{i}Mt}, \end{aligned} \tag{5.17}$$

completing the proof. Note that for convenience we ignore the fact that the spectrum of $M\tilde{t}$ may not be in $[0, 2\pi)$. This step will be justified in the next section.

By direct substitution one can verify that M has eigenvectors

$$\phi_{\pm}(0) = \sqrt{\tfrac{1}{2}}\begin{bmatrix} \pm 1 \\ 1 \end{bmatrix} \tag{5.18}$$

with eigenvalues $\frac{\omega}{2} \mp k$. Further,

$$\mathrm{i}Z^*\dot{Z} = \begin{bmatrix} \omega & 0 \\ 0 & 0 \end{bmatrix} \tag{5.19}$$

so that

$$\mathrm{i}\int_0^{\tilde{t}} Z^*\dot{Z}\,\mathrm{d}t = 2\pi\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{5.20}$$

Hence the cyclic initial states $\phi_{\pm}(0)$ have Berry phases

$$\begin{aligned} \gamma_{\pm} &= \mathrm{i}\int_0^{\tilde{t}} \langle \phi_{\pm}(0) \mid Z^*(t)\dot{Z}(t) \mid \phi_{\pm}(0)\rangle\,\mathrm{d}t \\ &= \pi, \end{aligned} \tag{5.21}$$

in agreement with the result obtained by the direct method of section 3.1. This simple example shows the compactness of Moore and Stedman's formalism as compared to the direct calculation of section 3.1.

5.2 Quasi-degeneracy

In the previous section I restricted $M\tilde{t}$ to have spectrum in $[0, 2\pi)$. At first sight, the only function of this restriction may seem to be to guarantee the uniqueness of the operators Z and M in the decomposition $U = Z\exp\{\mathrm{i}Mt\}$. In this section I will show that it has a deeper significance. We will see that requiring the spectrum of $M\tilde{t}$ to be in the half-open interval $[0, 2\pi)$ ensures that we find all of the cyclic initial states. Relaxing the restriction leads to the existence of an infinite set of pairs Z, M, with Z $\tilde{t}$-periodic and unitary and M constant and self-adjoint, such that $U = Z\exp\{\mathrm{i}Mt\}$. For most systems this redundancy is not important as all choices reproduce the same set of cyclic initial states. However if any two cyclic initial states are quasi-degenerate, that is if any two cyclic initial states have the same overall phase, then there will be choices of Z and M which do not give all of the cyclic initial states. This result can be used to explain how time-independent systems can have non-zero Berry phases [Moore 1990b].

Imagine that we have dropped the restriction on M. To see how quasi-degeneracy affects the formalism we must explicitly construct the set of pairs Z, M satisfying the other conditions. For notational clarity, I will reserve the symbols Z and M for the operators in the standard decomposition with $\sigma(M\tilde{t}) \subseteq [0, 2\pi)$. We can write the other choices that arise when the spectral condition is dropped as $Z' = ZK$ and $M' = M + L$ for some unitary K and self-adjoint L. As Z' is $\tilde{t}$-periodic and M' is constant, K must be $\tilde{t}$-periodic (with $K(0) = 1$) and L must be constant. Further, $U = Z\exp\{\mathrm{i}Mt\} = Z'\exp\{\mathrm{i}M't\}$. Hence

$$Z\mathrm{e}^{\mathrm{i}Mt} = ZK\mathrm{e}^{\mathrm{i}(M+L)t}. \tag{5.22}$$

Substituting $t = \tilde{t}$, and using the fact that $Z(\tilde{t}) = K(\tilde{t}) = 1$ gives

$$\mathrm{e}^{\mathrm{i}M\tilde{t}} = \mathrm{e}^{\mathrm{i}(M+L)\tilde{t}}. \tag{5.23}$$

For convenience, let there be a complete set of cyclic initial states, that is let M be diagonalisable. Put $M\tilde{t} = \sum_\alpha \chi_\alpha P_\alpha$, where P_α projects onto the cyclic initial state $\phi_\alpha(0)$.

Now it would be tempting to say that the $\phi_\alpha(0)$ must also be eigenvectors of $M + L$ and so of L itself, however this is not necessarily true. In fact it is this failure that makes the spectral condition $\sigma(M\tilde{t}) \subseteq [0, 2\pi)$ important. The $\phi_\alpha(0)$ are cyclic initial states because they are the eigenvectors of the monodromy operator $U(\tilde{t})$. If one of these eigenvectors is non-quasi-degenerate, that is it does not share its overall phase with any other linearly independent cyclic initial state, then it must be an eigenvector of $M\tilde{t}$ and so of M. Further, it must also be an eigenvector of L. However, not all cyclic initial states are necessarily non-quasi-degenerate. We will see in section 8.2 that there are systems for which all of the cyclic initial states are quasi-degenerate.

For simplicity, imagine that just two vectors $\phi_1(0)$ and $\phi_2(0)$ are quasi-degenerate, with overall phase χ. Then, due to the linearity of the evolution operator, any linear combination of them is also a cyclic initial state with overall phase χ. The problem is that condition (5.23) is satisfied if we choose L to be such that $L\phi_1(0) = 0$ and $L\phi_2(0) = 2\pi/\tilde{t}\phi_2(0)$. Then, while $\phi_1(0)$ and $\phi_2(0)$ are still eigenvectors of $M' = M + L$, it is no longer true that an arbitrary linear combination of them must also be one. In other words, due to the fact that the overall phase is only defined modulo 2π, not all cyclic initial states need to be eigenvectors of M'. However, as we have restricted the eigenvalues of $M\tilde{t}$ to be in the range $[0, 2\pi)$ this problem cannot occur for M. To summarise, the condition on the spectrum of $M\tilde{t}$ is necessary in order to find all of the cyclic initial states in systems which are quasi-degenerate.

Even though the cyclic initial states are not all eigenvectors of L, we can still find a complete set $\{\phi_\alpha(0)\}$ of them that are by careful choice within each quasi-degenerate eigenspace of $U(\tilde{t})$. To be consistent with equation (5.23), the corresponding eigenvalues of $L\tilde{t}$ must be integral multiples of 2π. We write $L = 2\pi N/\tilde{t}$ with $N = \sum_\alpha n_\alpha P_\alpha$, where the n_α are integers and P_α projects onto $\phi_\alpha(0)$. Finally, this can be consistent with equation (5.22) iff we take $K = \exp\{-2\pi i N t/\tilde{t}\}$. In other words, if we drop the restriction on the spectrum of $M\tilde{t}$, we are left with an infinite set of $\tilde{t}$-periodic unitary Z' and constant self-adjoint M' satisfying

$U = Z'\exp\{\mathrm{i}M't\}$. These operators are related to the standard pair Z, M by

$$Z' = Z\mathrm{e}^{-2\pi\mathrm{i}Nt/\tilde{t}}, \tag{5.24}$$

$$M' = M + 2\pi N/\tilde{t}, \tag{5.25}$$

where N commutes with M and has integral eigenvalues.

As we have seen, the pairs Z', M' cannot be used for quasi-degenerate cyclic initial states. Nevertheless, I will now show that they can be used for non-quasi-degenerate systems. This justifies the dropping of the spectral condition in the example of the last section. Let $\phi(0)$ be a non-quasi-degenerate cyclic initial state with overall phase χ and $M' = M + 2\pi N/\tilde{t}$ be such that $N\phi(0) = n\phi(0)$ for some integer n. Then $\phi(0)$ is indeed an eigenvector of M'. Further, the overall phase is the corresponding eigenvalue of $M'\tilde{t}$ (modulo 2π). Thus we need merely show that equation (5.11) applied to Z' gives the correct Berry phase. By direct substitution we have

$$Z'^*\dot{Z}' = \mathrm{e}^{2\pi\mathrm{i}Nt/\tilde{t}}\left(Z^*\dot{Z} - 2\pi\mathrm{i}N/\tilde{t}\right)\mathrm{e}^{-2\pi\mathrm{i}Nt/\tilde{t}}. \tag{5.26}$$

$$\begin{aligned}\Rightarrow \qquad \gamma' &= \mathrm{i}\int_0^{\tilde{t}} \langle\phi(0) \mid Z'^*\dot{Z}' \mid \phi(0)\rangle \,\mathrm{d}t \\ &= \mathrm{i}\int_0^{\tilde{t}} \langle\phi(0) \mid Z^*\dot{Z} - 2\pi\mathrm{i}n/\tilde{t} \mid \phi(0)\rangle \,\mathrm{d}t \\ &= \gamma + 2n\pi. \end{aligned} \tag{5.27}$$

Thus we recover the Berry phase (modulo 2π) as required.

This result can be used to calculate the Berry phases for time-independent systems. These are important as all isolated systems have constant Hamiltonians. Let H be a constant Hamiltonian. Then we can regard H as being periodic with arbitrary period $\tilde{t}$. As we shall see, it is only for special values of $\tilde{t}$ that non-zero Berry phases are possible. For these systems the evolution operator is given by $U = \exp\{-\mathrm{i}Ht\}$. Thus we can take $Z' = 1$ and $M' = -H$. Ignoring quasi-degeneracy for the moment, this means that the eigenvectors of H are cyclic initial states for any period $\tilde{t}$. As mentioned in section 2.1, it is this behaviour that leads

to them being called stationary states. However, as Z' is constant, $Z'^*\dot{Z}' = 0$ so that the Berry phases are all zero. This is to be expected, as the definition of the dynamical phase is motivated by the phase evolution in the time-independent case.

However, given any two eigenvectors $\phi_1(0)$ and $\phi_2(0)$ of H, with energies E_1 and E_2 repectively, we can choose the period $\tilde{t}$ in such a way that $\phi_1(0)$ and $\phi_2(0)$ become quasi-degenerate. For example, assuming that $E_2 > E_1$, take

$$\tilde{t} = 2\pi(E_2 - E_1)^{-1}. \tag{5.28}$$

Then

$$M'\tilde{t}\phi_1(0) = -\frac{2\pi E_1}{E_2 - E_1}\phi_1(0), \tag{5.29}$$

$$\begin{aligned} M'\tilde{t}\phi_2(0) &= -\frac{2\pi E_2}{E_2 - E_1}\phi_2(0) \\ &= -\left(2\pi + \frac{2\pi E_1}{E_2 - E_1}\right)\phi_2(0). \end{aligned} \tag{5.30}$$

Hence $\phi_1(0)$ and $\phi_2(0)$ are quasi-degenerate, having the common overall phase $\chi = -2\pi E_1(E_2 - E_1)^{-1}$. This means that any linear combination

$$\phi(0) = a_1\phi_1(0) + a_2\phi_2(0) \tag{5.31}$$

is also a cyclic initial state with overall phase χ. However, in general $\phi(0)$ will not be an eigenvector of H and so will not be barred from having a non-trivial Berry phase. To calculate this phase we need the standard Z and M. We try the transformations (5.24) and (5.25) with $n_1 = 0$ and $n_2 = -1$. Then

$$M\tilde{t}\phi_1(0) = -\frac{2\pi E_1}{E_2 - E_1}\phi_1(0), \tag{5.32}$$

$$\begin{aligned} M\tilde{t}\phi_2(0) &= M'\tilde{t}\phi_2(0) + 2\pi\phi_2(0) \\ &= -\frac{2\pi E_1}{E_2 - E_1}\phi_2(0), \end{aligned} \tag{5.33}$$

confirming our choice. To find the Berry phases we need $Z^*\dot{Z}$. As $Z' = 1$ we have that $Z = \exp\{2\pi\mathrm{i}Nt/\tilde{t}\}$. Thus $Z^*\dot{Z} = 2\pi\mathrm{i}N/\tilde{t}$, giving $\mathrm{i}\int_0^{\tilde{t}} Z^*\dot{Z}\,\mathrm{d}t = -2\pi N$. Substituting into equation (5.11) and using the fact that $N\phi_1(0) = 0$ and $N\phi_2(0) =$

$-\phi_2(0)$ we find that

$$\begin{aligned}\gamma &= -2\pi\langle\phi(0) \mid N \mid \phi(0)\rangle \\ &= 2\pi|a_2|^2,\end{aligned} \tag{5.34}$$

in agreement with Moore and Stedman [1990b].

We may use this general result to rederive the Berry phases for the Hamiltonian

$$H = -\mu B\sigma_z \tag{5.35}$$

discussed by Aharonov and Anandan [1987]. This has eigenvectors

$$\phi_1(0) = \begin{bmatrix}1\\0\end{bmatrix}, \tag{5.36}$$

$$\phi_2(0) = \begin{bmatrix}0\\1\end{bmatrix}, \tag{5.37}$$

with energies $E_1 = -\mu B$ and $E_2 = \mu B$ respectively. Thus to get non-zero Berry phases we must choose $\tilde{t} = \pi/\mu B$. Applying equation (5.34), the arbitrary cyclic initial state

$$\phi(0) = \begin{bmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}\end{bmatrix} \tag{5.38}$$

has Berry phase

$$\gamma = \pi(1 - \cos\theta), \tag{5.39}$$

in agreement with the previous authors.

Thus we have seen that Berry phases for time-independent systems arise for a different reason than those for time-dependent systems. For time-dependent systems a period is forced onto us by the periodicity of the Hamiltonian, and the Berry phases arise due to the time dependence behind that periodicity. In contrast, for time-independent systems we can choose any period, and it is only for certain judicious choices (those which make two stationary states quasi-degenerate) that non-zero Berry phases are possible.

As a further example, consider time-dependent Hamiltonians that commute with themselves, that is Hamiltonians for which $[H(t'), H(t'')] = 0$ for all t', t''. This condition means that $H(t)$ commutes with the integral $\int_0^t H(t')\,\mathrm{d}t'$ for all times. Hence

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\exp\{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'\} = -\mathrm{i}H(t)\exp\{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'\}. \tag{5.40}$$

But this is precisely the time-dependent Schrödinger equation – the equation that the evolution operator must satisfy. Hence

$$U(t) = \exp\{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'\}. \tag{5.41}$$

It is easy to verify that we can then take

$$Z' = \exp\{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'\}\exp\{\tfrac{\mathrm{i}t}{\tilde{t}}\int_0^{\tilde{t}} H(t')\,\mathrm{d}t'\}, \tag{5.42}$$

$$M' = -\frac{1}{\tilde{t}}\int_0^{\tilde{t}} H(t')\,\mathrm{d}t'. \tag{5.43}$$

But then

$$Z'^{*}\dot{Z}' = -\mathrm{i}H(t) + \tfrac{\mathrm{i}}{\tilde{t}}\int_0^{\tilde{t}} H(t')\,\mathrm{d}t', \tag{5.44}$$

which in turn implies that $\int_0^{\tilde{t}} Z'^{*}\dot{Z}'\,\mathrm{d}t = 0$. Hence non-zero Berry phases can only be obtained for quasi-degenerate systems.

Note that the time-dependent case is an example of this type. A simple example of a self-commuting Hamiltonian is a spin-j particle in a magnetic field of constant direction but changing magnitude [Sakurai 1985, p73]. This system has Hamiltonian $H(t) = \Omega(t)\mathbf{b}\cdot\mathbf{j}$ so that the evolution operator is given by $U(t) = \exp\{-\int_0^t \Omega(t')\,\mathrm{d}t'\mathbf{b}\cdot\mathbf{j}\}$. There is less scope for using quasi-degeneracy in these systems than for the time-independent ones discussed earlier. This is because the period $\tilde{t}$ is constrained by the period of the Hamiltonian, and so cannot be chosen to give a quasi-degeneracy. Hence any quasi-degeneracy must be naturally occurring.

5.3 Salzman's decomposition

For most systems, one must calculate the evolution operator before using Moore and Stedman's formalism. However, for some special cases this is not necessary, greatly simplifying the results of our treatment. In this section I discuss one class of such systems. This class includes the semi-classical Jaynes-Cummings model as well as the cranked Hamiltonians analysed by Wang [1990a, 1990b] and so is of some practical import. For these systems the single-valued vectors can be found by inspection once the Hamiltonian has been cast into a suitable form. Thus a suitable evolution operator decomposition can be found directly from the Hamiltonian, without having to display the evolution operator explicitly first. This decomposition was first discussed by Salzman [1974] and was used in the study of Berry phases by Moore [1990c].

Consider a time-dependent Hamiltonian that can be written in the form

$$H(t) = \mathrm{e}^{-\mathrm{i}At}\tilde{H}\mathrm{e}^{\mathrm{i}At}, \tag{5.45}$$

with A and $\tilde{H}$ constant. Obviously a necessary but not sufficient condition is that H must have time-independent eigenvalues. Now define the operator U by

$$U(t) = \mathrm{e}^{-\mathrm{i}At}\mathrm{e}^{-\mathrm{i}Bt}, \tag{5.46}$$

where $B = \tilde{H} - A$ is a time-independent self-adjoint operator. Then

$$\begin{aligned} \mathrm{i}\dot{U} &= \mathrm{e}^{-\mathrm{i}At}(A+B)\mathrm{e}^{-\mathrm{i}Bt} \\ &= \mathrm{e}^{-\mathrm{i}At}(A+B)\mathrm{e}^{\mathrm{i}At}\mathrm{e}^{-\mathrm{i}At}\mathrm{e}^{-\mathrm{i}Bt} \\ &= HU. \end{aligned} \tag{5.47}$$

Thus U is indeed the evolution operator corresponding to the Hamiltonian H. This is the operator decomposition we require.

Now imagine that H is $\tilde{t}$-periodic: $H(\tilde{t}) = H(0)$. Then as

$$H(\tilde{t}) = A + \mathrm{e}^{-\mathrm{i}A\tilde{t}}B\mathrm{e}^{-\mathrm{i}A\tilde{t}} \tag{5.48}$$

and

$$H(0) = A + B, \tag{5.49}$$

we can see that H is $\tilde{t}$-periodic iff $\exp\{-\mathrm{i}A\tilde{t}\}$ commutes with B. Thus $\exp\{-\mathrm{i}A\tilde{t}\}$ and B have a complete set of simultaneous eigenvectors $\phi_\alpha(0)$ (assuming for simplicity that there is a complete set of cyclic initial states). Later we will verify that the $\phi_\alpha(0)$ are indeed cyclic initial states. Let

$$B\phi_\alpha(0) = B_\alpha\phi_\alpha(0), \tag{5.50}$$

$$\mathrm{e}^{-\mathrm{i}A\tilde{t}}\phi_\alpha(0) = \mathrm{e}^{-\mathrm{i}\theta_\alpha}\phi_\alpha(0). \tag{5.51}$$

We note that, while $\exp\{-\mathrm{i}A\tilde{t}\}$ and B commute, A and B do not necessarily commute. In fact if they do, the Hamiltonian (5.45) will be time-independent. Now the monodromy operator $U(\tilde{t})$ is given by $U(\tilde{t}) = \exp\{-\mathrm{i}A\tilde{t}\}\exp\{-\mathrm{i}B\tilde{t}\}$ so that

$$U(\tilde{t})\phi_\alpha(0) = \mathrm{e}^{-\mathrm{i}\theta_\alpha}\mathrm{e}^{-\mathrm{i}B_\alpha\tilde{t}}\phi_\alpha(0). \tag{5.52}$$

Thus the vectors $\phi_\alpha(0)$ are indeed cyclic initial states with overall phases $\chi_\alpha = -(\theta_\alpha + B_\alpha\tilde{t})$.

To calculate the corresponding Berry phases we calculate the dynamical phase δ_α directly. For this class of systems, this turns out to be easier than finding a single-valued vector. We have

$$\begin{aligned}
\delta_\alpha &= -\int_0^{\tilde{t}} \langle\phi_\alpha(0) \mid U^*(t)H(t)U(t) \mid \phi_\alpha(0)\rangle \,\mathrm{d}t \\
&= -\int_0^{\tilde{t}} \langle\phi_\alpha(0) \mid \mathrm{e}^{\mathrm{i}Bt}(A+B)\mathrm{e}^{-\mathrm{i}Bt} \mid \phi_\alpha(0)\rangle \,\mathrm{d}t \\
&= -B_\alpha\tilde{t} - \langle\phi_\alpha(0) \mid A \mid \phi_\alpha(0)\rangle\tilde{t}.
\end{aligned} \tag{5.53}$$

Thus the cyclic initial states $\phi_\alpha(0)$ have Berry phases

$$\begin{aligned}
\gamma_\alpha &= \chi_\alpha - \delta_\alpha \\
&= \langle\phi_\alpha(0) \mid A \mid \phi_\alpha(0)\rangle\tilde{t} - \theta_\alpha.
\end{aligned} \tag{5.54}$$

Note that if the Hamiltonian is time-independent then, barring any problems due to quasi-degeneracy, $\phi_\alpha(0)$ is an eigenvector of A with eigenvalue $\theta_\alpha/\tilde{t}$. Hence equation (5.54) gives the Berry phases as zero in agreement with the discussion in section 5.2 above.

This formalism can easily be connected to that of Moore and Stedman. If $\exp\{-\mathrm{i}A\tilde{t}\}$ was unity then, again barring any complications due to quasi-degeneracy, we could take $Z = \exp\{-\mathrm{i}At\}$ and $M = -B$. The situation is not much more complicated in general. Let Θ be the operator with eigenvectors $\phi_\alpha(0)$ (the eigenvectors of B) and eigenvalues θ_α. Then by comparing the forms of the evolution operator $U = Z\exp\{\mathrm{i}Mt\}$ and $U = \exp\{-\mathrm{i}At\}\exp\{-\mathrm{i}Bt\}$ and noting that Θ and B commute (as they have the same eigenvectors), one can easily show that

$$Z = \mathrm{e}^{-\mathrm{i}At}\mathrm{e}^{\mathrm{i}\Theta t/\tilde{t}}, \tag{5.55}$$

$$M = -B - \Theta/\tilde{t}. \tag{5.56}$$

Hence the decomposition of Moore and Stedman can be recovered from that of Salzman.

This formalism can be used to calculate the Berry phases for spherically symmetric atoms in semi-classical circularly polarised radiation fields. Further, we can take the two-level limit and verify that we reproduce the results obtained earlier by different methods. With $k = \omega/c$, let the field have vector potential [Salzman 1974]

$$\mathbf{A} = \frac{E_0 c}{\omega}(\cos(kz - \omega t), \sin(kz - \omega t), 0)\,. \tag{5.57}$$

Thus, as p_x and p_y commute with functions of z and t, the Hamiltonian is given by

$$\begin{aligned} H(t) &= H_0 - \frac{e}{2mc}\mathbf{p}\cdot\mathbf{A} - \frac{e}{2mc}\mathbf{A}\cdot\mathbf{p} + \frac{e^2}{2mc^2}\mathbf{A}^2 \\ &= H_0 - \frac{eE_0}{m\omega}(p_x\cos(kz - \omega t) + p_y\sin(kz - \omega t)) + \frac{e^2E_0^2}{2m\omega^2}, \end{aligned} \tag{5.58}$$

where H_0 is the spherically symmetric unperturbed atomic Hamiltonian.

We need to simplify the expression $p_x \cos(kz-\omega t)+p_y \sin(kz-\omega t)$ in equation (5.58). Define the operator $X(\theta) = p_x \cos\theta + p_y \sin\theta$. Then, using the fact that $[p_x, L_z] = -\mathrm{i}p_y$ and $[p_y, L_z] = \mathrm{i}p_x$, we have

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\theta}X &= -p_x \sin\theta + p_y \cos\theta \\ &= \mathrm{i}[p_y, L_z]\sin\theta + \mathrm{i}[p_x, L_z]\cos\theta \\ &= \mathrm{i}[X, L_z]. \end{aligned} \tag{5.59}$$

Now consider the operator $Y(\theta) = \exp\{-\mathrm{i}\theta L_z\} p_x \exp\{\mathrm{i}\theta L_z\}$. We have

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\theta}Y &= -\mathrm{i}L_z \mathrm{e}^{-\mathrm{i}\theta L_z} p_x \mathrm{e}^{\mathrm{i}\theta L_z} + \mathrm{i}\mathrm{e}^{-\mathrm{i}\theta L_z} p_x \mathrm{e}^{\mathrm{i}\theta L_z} L_z \\ &= \mathrm{i}[Y, L_z]. \end{aligned} \tag{5.60}$$

Further, $X(0) = Y(0) = p_x$ so that X and Y solve the same initial value problem. But the solution of a linear initial value problem is unique and so X and Y are equal. In other words,

$$\mathrm{e}^{-\mathrm{i}\theta L_z} p_x \mathrm{e}^{\mathrm{i}\theta L_z} = p_x \cos\theta + p_y \sin\theta. \tag{5.61}$$

This is the simplification we need. Now, as H_0 is assumed to be spherically symmetric, it commutes with L_z. This means that, substituting $\theta = kz - \omega t$ into equation (5.61), we can write the Hamiltonian (5.58) in the form

$$H(t) = \mathrm{e}^{-\mathrm{i}(kz-\omega t)L_z}\left(H_0 - \frac{eE_0}{m\omega}p_x + \frac{e^2E_0^2}{2m\omega^2}\right)\mathrm{e}^{\mathrm{i}(kz-\omega t)L_z}. \tag{5.62}$$

In the electric dipole approximation we ignore the kz factors giving finally

$$H(t) = \mathrm{e}^{\mathrm{i}\omega t L_z}\left(H_0 - \frac{eE_0}{m\omega}p_x + \frac{e^2E_0^2}{2m\omega^2}\right)\mathrm{e}^{-\mathrm{i}\omega t L_z}. \tag{5.63}$$

This is of the form (5.45) and the Hamiltonian is $\tilde{t} = 2\pi/\omega$-periodic. Thus we can find the atomic cyclic initial states and Berry phases using the formalism developed above. By inspection we have

$$A = -\omega L_z, \tag{5.64}$$

$$B = H_0 + \omega L_z - \frac{eE_0}{m\omega}p_x + \frac{e^2E_0^2}{2m\omega^2}. \tag{5.65}$$

To evaluate $\exp\{-\mathrm{i}A\tilde{t}\}$ we work in the basis $\{|\ lm\rangle\}$ of joint eigenvectors of L^2 and L_z. Then, using the fact that $\omega\tilde{t} = 2\pi$, we have that

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}A\tilde{t}}\ |\ lm\rangle &= \mathrm{e}^{2\pi\mathrm{i}L_z}\ |\ lm\rangle \\ &= \mathrm{e}^{2\mathrm{i}m\pi}\ |\ lm\rangle \\ &= |\ lm\rangle. \end{aligned} \tag{5.66}$$

Thus, as $\exp\{-\mathrm{i}A\tilde{t}\} = 1$, the θ_α are all zero and, from equation (5.54), the Berry phases for the cyclic initial states $\phi_\alpha(0)$ (the eigenvectors of B) are simply given by

$$\gamma_\alpha = -2\pi\langle\phi_\alpha(0)\ |\ L_z\ |\ \phi_\alpha(0)\rangle. \tag{5.67}$$

This result can be used to examine the two-level atomic limit. In this approximation the cyclic initial states $\phi_\alpha(0)$ are taken to be linear combinations of the two relevant atomic states, say $|\ n_\pm l_\pm m_\pm\rangle$. That is,

$$\phi_\pm(0) = y_\pm\ |\ n_+ l_+ m_+\rangle + x_\pm\ |\ n_- l_- m_-\rangle. \tag{5.68}$$

Now the selection rules [Woodgate 1986, p46] require $m_+ = m_- + 1$ so that

$$\begin{aligned} \gamma_\pm &= -2\pi\langle\phi_\pm(0)\ |\ L_z\ |\ \phi_\pm(0)\rangle \\ &= 2\pi|x_\pm|^2, \end{aligned} \tag{5.69}$$

in agreement with the previous calculations.

Another instructive example is a spin-j particle in a rotating magnetic field $\mathbf{b}(t)$. The field is written in lower case to distinguish it from the operator B in the decomposition (5.46). The system has Hamiltonian

$$H(t) = \mathbf{b}(t)\cdot\mathbf{j}, \tag{5.70}$$

where $[j_x, j_y] = j_z$. Now consider the magnetic field [Wang 1990a]

$$\mathbf{b}(t) = \Omega\left(\sin\theta\cos\omega t, \sin\theta\sin\omega t, \cos\theta\right). \tag{5.71}$$

Then H is $\tilde{t}$-periodic with $\tilde{t} = 2\pi/\omega$. We must cast H into the form (5.45). Note that throughout this example I will be using identities of the form

$$e^{-i\theta j_y} j_z e^{i\theta j_y} = j_x \sin\theta + j_z \cos\theta. \tag{5.72}$$

These can be proved in the same way as was equation (5.61). We try the operator $H(t) = \exp\{-ij_z\omega t\}H(0)\exp\{ij_z\omega t\}$. Expanding, we have

$$\begin{aligned} H(t) &= \Omega \sin\theta e^{-ij_z\omega t} j_x e^{ij_z\omega t} + \Omega\cos\theta e^{-ij_z\omega t} j_z e^{ij_z\omega t} \\ &= \Omega\sin\theta\,(\cos\omega t j_x + \sin\omega t j_y) + \Omega\cos\theta j_z \\ &= \mathbf{b}(t)\cdot\mathbf{j}, \end{aligned} \tag{5.73}$$

verifying our choice. Thus the Hamiltonian is of the form (5.45), with

$$A = \omega j_z, \tag{5.74}$$

$$B = H(0) - \omega j_z. \tag{5.75}$$

To get the Berry phases we first need the cyclic initial states, that is the eigenvectors of B. We try

$$\phi_m(0) = e^{-i\bar{\theta} j_y} \mid jm\rangle, \tag{5.76}$$

where

$$\sin\bar{\theta} = \frac{\sin\theta}{[1 - 2\omega/\Omega\cos\theta + \omega^2/\Omega^2]^{1/2}}, \tag{5.77}$$

$$\cos\bar{\theta} = \frac{\cos\theta - \omega/\Omega}{[1 - 2\omega/\Omega\cos\theta + \omega^2/\Omega^2]^{1/2}}. \tag{5.78}$$

By direct substitution we have

$$\begin{aligned} B\phi_m(0) &= \Omega e^{-i\bar{\theta}j_y} e^{i\bar{\theta}j_y} \left(j_x\sin\theta + j_z(\cos\theta - \omega/\Omega)\right) e^{-i\bar{\theta}j_y} \mid jm\rangle \\ &= \Omega e^{-i\bar{\theta}j_y} \Big(\big(j_x \left(\sin\theta\cos\bar{\theta} - \sin\bar{\theta}(\cos\theta - \omega/\Omega)\right) \\ &\qquad + j_z \left(\sin\theta\sin\bar{\theta} + \cos\bar{\theta}(\cos\theta - \omega/\Omega)\right)\big) \mid jm\rangle \\ &= \Omega e^{-i\bar{\theta}j_y} j_z \mid jm\rangle \\ &= m\Omega\phi_m(0). \end{aligned} \tag{5.79}$$

Hence $\phi_m(0)$ is indeed an eigenvector of B with eigenvalue $B_\alpha = m\Omega$. Now $\exp\{-\mathrm{i}A\tilde{t}\}$ is unity so that the θ_α in equation (5.54) are all zero. Thus the Berry phases are

$$\begin{aligned}\gamma_m &= 2\pi\langle jm \mid \mathrm{e}^{\mathrm{i}\overline{\theta}j_y} j_z \mathrm{e}^{-\mathrm{i}\overline{\theta}j_y} \mid jm\rangle \\ &= 2\pi\langle jm \mid -j_x \sin\overline{\theta} + j_z \cos\overline{\theta} \mid jm\rangle \\ &= 2m\pi\cos\overline{\theta}, \end{aligned} \tag{5.80}$$

in agreement with Wang [1990a].

5.4 Cheng and Fung's decomposition

I will discuss one more decomposition formalism. It is a modification of the work of Cheng and Fung [1989]. This approach is interesting as it is very general, encompassing both of the methods already discussed in this chapter. However its very generality makes it calculationally inefficient as the cyclic initial states must be found by some other method before the decomposition can be found. Further, Cheng and Fung's method is only valid if there is a complete set of cyclic initial states. As we shall see in section 8.1, this is not a problem for finite dimensional Hilbert spaces, but is by no means guaranteed in general.

Let the $\tilde{t}$-periodic Hamiltonian H have a complete set of cyclic initial states $\phi_\alpha(0)$. We decompose the evolution operator as in equation (5.1) into the form $U(t) = \mathbf{U}(t)\mathbf{R}(t)$. We merely require that $\mathbf{U}$ and $\mathbf{R}$ be unitary with $\mathbf{U}(0) = \mathbf{R}(0) = 1$, and that $\mathbf{R}(t)$ be diagonal in the basis $\{\phi_\alpha(0)\}$ at all times. Put $\mathbf{R}(t)\phi_\alpha(0) = \exp\{\mathrm{i}\theta_\alpha\}\phi_\alpha(0)$. Then θ_α is real as $\mathbf{R}$ is unitary, and we may take $\theta_\alpha(0)$ as $\mathbf{R}(0) = 1$. The decomposition of Moore and Stedman is of this type (with $\mathbf{U} = Z$ and $\mathbf{R} = \exp\{\mathrm{i}Mt\}$) as is that of Salzman (with $\mathbf{U} = \exp\{-\mathrm{i}At\}$ and $\mathbf{R} = \exp\{-\mathrm{i}Bt\}$). However note that neither of these decompositions require the existence of a complete set of cyclic initial states. Now, let the system start in the state $\phi_\alpha(0)$. This evolves into

$$\begin{aligned}\phi_\alpha(t) &= \mathbf{U}(t)\mathbf{R}(t)\phi_\alpha(0) \\ &= \mathrm{e}^{\mathrm{i}\theta_\alpha(t)}\mathbf{U}(t)\phi_\alpha(0). \end{aligned} \tag{5.81}$$

In particular, at $t = \tilde{t}$, $\phi_\alpha(\tilde{t}) = \exp\{\mathrm{i}\theta_\alpha(\tilde{t})\}\mathbf{U}(\tilde{t})\phi_\alpha(0)$. However $\phi_\alpha(0)$ is a cyclic initial state so that $\phi_\alpha(\tilde{t}) = \exp\{\mathrm{i}\chi_\alpha\}\phi_\alpha(0)$. Hence $\phi_\alpha(0)$ must be an eigenvector of $\mathbf{U}(\tilde{t})$. Putting $\mathbf{U}(\tilde{t})\phi_\alpha(0) = \exp\{\mathrm{i}\lambda_\alpha\}\phi_\alpha(0)$, we have $\chi_\alpha = \lambda_\alpha + \theta_\alpha(\tilde{t})$. Note that if we put $\mathbf{U} = Z$ and $\mathbf{R} = \exp\{\mathrm{i}Mt\}$ then the λ_α are all zero and the overall phases are just $\chi_\alpha = \theta_\alpha(\tilde{t})$.

To find the Berry phases we must investigate the nature of $\theta_\alpha(\tilde{t})$ more closely. We have

$$\begin{aligned}
& \mathrm{i}\dot{\phi}_\alpha(t) = H(t)\phi_\alpha(t) \\
\Rightarrow \quad & \mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t}\left(\mathrm{e}^{\mathrm{i}\theta_\alpha}\mathbf{U}\phi_\alpha(0)\right) = H\mathrm{e}^{\mathrm{i}\theta_\alpha}\mathbf{U}\phi_\alpha(0) \\
\Rightarrow \quad & H\mathbf{U}\phi_\alpha(0) = -\dot{\theta}_\alpha\mathbf{U}\phi_\alpha(0) + \mathrm{i}\dot{\mathbf{U}}\phi_\alpha(0) \\
\Rightarrow \quad & \dot{\theta}_\alpha = \mathrm{i}\langle\phi_\alpha(0) \mid \mathbf{U}^*\dot{\mathbf{U}} - \mathbf{U}^*H\mathbf{U} \mid \phi_\alpha(0)\rangle \\
\Rightarrow \quad & \theta_\alpha = \Gamma_\alpha + \delta_\alpha, \qquad (5.82)
\end{aligned}$$

where $\delta_\alpha = -\int_0^{\tilde{t}}\langle\psi_\alpha(0) \mid U^*HU \mid \phi_\alpha(0)\rangle\,\mathrm{d}t$ is the usual dynamical phase and $\Gamma_\alpha = \mathrm{i}\int_0^{\tilde{t}}\langle\phi_\alpha(0) \mid \mathbf{U}^*\dot{\mathbf{U}} \mid \phi_\alpha(0)\rangle\,\mathrm{d}t$ is a topological phase. Note that we can replace $\mathbf{U}$ in the expression for the dynamical phase with U because the states $\phi_\alpha(0)$ are eigenvectors of $\mathbf{R}$. Thus we can put a factor of $\mathbf{R}^*$ at the start of the operator inside the inner product and a factor of $\mathbf{R}$ at the end without altering the value of the inner product, the two introduced phases cancelling. Hence, as the overall phase is given by $\chi_\alpha = \theta_\alpha + \lambda_\alpha$, the Berry phase is given by

$$\gamma_\alpha = \Gamma_\alpha + \lambda_\alpha. \qquad (5.83)$$

Thus the Berry phase is partitioned into the sum of two parts, as was the case with Salzman's decomposition. Note that if we put $\mathbf{U} = Z$ and $\mathbf{R} = \exp\{\mathrm{i}Mt\}$ we recover the expression (5.11) for the Berry phase.

Hence the decomposition of Moore and Stedman is a special case of the one of Cheng and Fung with the following useful features: the extra term λ_α in the Berry phase is zero, displaying the Berry phase more clearly, and the decomposition can be achieved without first finding the cyclic initial states from the evolution

operator. This program of streamlining the calculational algorithm is carried further in the next chapter. There I show how to calculate the Berry phases directly from the Fourier decomposition of the Hamiltonian, without having to find the evolution operator first. Finally the formalism of Moore and Stedman does not require the existence of a complete set of cyclic initial states.

Chapter Six

Fourier theory

The formalism presented in the last chapter is very useful for simple examples, such as the two-level atom, and for providing a framework in which new results can be obtained. For example, in section 8.3 I use it to investigate the existence of cyclic initial states. However, in most cases one must still calculate the evolution operator before finding the operators Z and M, an obvious exception being the Hamiltonians discussed in section 5.3. In this chapter I show how to evaluate the cyclic initial states and Berry phases without having to expend this computational effort. This is achieved by transforming the time-dependent problem into an equivalent time-independent one. To do this we must work in a new Hilbert space, which is infinite-dimensional even if the original one is not. This approach was first used in the investigation of periodic systems by Shirley [1965] and applied to the calculation of Berry phases by Moore [1990a].

The extra difficulty caused by this expansion of the Hilbert space is more than compensated for by the effective time-independence of the restated problem. Instead of having to solve the time-dependent Schrödinger equation explicitly, we need merely find the eigenvectors of a certain operator, the Floquet Hamiltonian, that is defined on the new Hilbert space. Further advantages over the direct method accrue when the system is not exactly solvable, for then we may use the powerful techniques of time-independent perturbation theory.

By rewriting the Floquet Hamiltonian as a matrix in a given basis, the method used by Shirley, strong links can be forged between this formalism and that of Moore and Stedman (which was discussed in section 5.1). This reformulation utilises the Fourier decomposition of the Hamiltonian, effectively solving the evo-

lution equation Fourier component by Fourier component. In section 9.1 I will show how the Fourier method allows us to relate the Berry phases for the Jaynes-Cummings model to the (measurable) Rabi oscillations.

6.1 The Floquet Hamiltonian

We need a few preliminary results. Let the quantum system of interest have Hilbert space $\mathcal{H}$. For example, a single non-relativistic particle has Hilbert space $L^2(\mathbb{R}, \mathrm{d}^3x)$. We take $\mathcal{H}$ to have inner product $\langle \cdot \mid \cdot \rangle$ and basis $\{\xi_\alpha\}$. We also introduce the Hilbert space $\mathcal{T}$ of $\tilde{t}$-periodic functions $f : \mathbb{R} \to \mathbb{C}$ with inner product $(f \mid g) = (1/\tilde{t}) \int_0^{\tilde{t}} \overline{f}(t) g(t)\, \mathrm{d}t$ and basis $\{\exp\{\mathrm{i}\omega t\}\}$, where $\omega = 2\pi/\tilde{t}$. In simple terms, $\mathcal{T}$ is the set of Fourier components. As we shall see, this identification is the cornerstone of the Fourier method.

Of interest here is the product Hilbert space $\mathcal{K} = \mathcal{T} \otimes \mathcal{H}$ first used by Sambe [1973]. This has basis $\{\exp\{\mathrm{i}\omega t\}\xi_\alpha\}$ and inner product $\langle\langle \cdot \mid \cdot \rangle\rangle = (1/\tilde{t}) \int_0^{\tilde{t}} \langle \cdot \mid \cdot \rangle \, \mathrm{d}t$. For convenience I will often write the basis elements of $\mathcal{H}$, $\mathcal{T}$ and $\mathcal{K}$ as $\mid \alpha\rangle$, $\mid n\rangle$ and $\mid \alpha n\rangle\rangle$ respectively. This space is important due to its close relation to the vector space $\mathcal{S}$ of single-valued vectors $\psi : \mathbb{R} \to \mathcal{H} : \psi(\tilde{t}) = \psi(0)$. In fact, $\mathcal{K}$ and $\mathcal{S}$ are isomorphic as vector spaces under the mapping

$$i : \mathcal{K} \to \mathcal{S} : \sum_{\alpha n} a_{\alpha n} \mid \alpha n\rangle\rangle \mapsto \sum_{\alpha} \sum_{n} a_{\alpha n} \exp\{\mathrm{i}n\omega t\} \mid \alpha\rangle. \tag{6.1}$$

Hence the single-valued vectors, which are the quantities needed to calculate the Berry phases, can be regarded as vectors in the direct product Hilbert space $\mathcal{K}$. This means that the vectors in $\mathcal{T}$ serve to provide the $\tilde{t}$-periodic time dependence of the single-valued vectors. It is in this sense that $\mathcal{T}$ can be regarded as the set of Fourier components. In the following we use this identification to display the single-valued vectors as the eigenvectors of a certain operator, the Floquet Hamiltonian defined on $\mathcal{K}$. This reduces the problem from solving the time-dependent Schrödinger equation in $\mathcal{H}$ to solving an eigenvector equation in $\mathcal{K}$. In other words we have transformed the time-dependent problem into an equivalent

time-independent one where, as noted by Casati and Molinari [1989], the Floquet Hamiltonian plays the part of the system's Hamiltonian.

To find the form of the Floquet Hamiltonian, we use the special single-valued vectors $\psi_\alpha(t) = Z(t)\phi_\alpha(0)$ of Moore and Stedman's formalism. As mentioned in the section 5.1, these are the vectors with the simplest phase relationship to the evolving state $\phi_\alpha(t)$. We have

$$\phi_\alpha(t) = \mathrm{e}^{\mathrm{i}\chi_\alpha t/\tilde{t}}\psi_\alpha(t), \tag{6.2}$$

where the cyclic initial state $\phi_\alpha(0)$ has overall phase χ_α. Substituting into the time-dependent Schrödinger equation gives

$$\begin{aligned} \mathrm{i}\dot{\phi}_\alpha &= H\phi_\alpha \\ \Rightarrow \qquad \left(H - \mathrm{i}\tfrac{\partial}{\partial t}\right)\psi_\alpha &= -\frac{\chi_\alpha}{\tilde{t}}\psi_\alpha. \end{aligned} \tag{6.3}$$

If we now regard $\psi_\alpha(t)$ as a vector in $\mathcal{K}$, we can identify equation (6.3) as an eigenvector equation,

$$K\psi_\alpha = \epsilon_\alpha\psi_\alpha, \tag{6.4}$$

where

$$K = H(t) - \mathrm{i}\tfrac{\partial}{\partial t} \tag{6.5}$$

is the Floquet Hamiltonian and $\epsilon = -\chi_\alpha/\tilde{t}$. Hence this formalism is closely related to that of Moore and Stedman. In the physical literature ϵ_α is often called a quasi-energy and ψ_α a quasi-energy state. [Zel'dovich 1967]. Hence the problem is reduced to finding the eigenvectors of K. In the next section the problem will be further simplified by using a matrix formulation. This exploits the Fourier decomposition of the Hamiltonian and leads to the results of Shirley [1965]. Further, the matrix formulation strengthens the relationship between this formalism and that of Moore and Stedman.

For the moment however, we continue with the formal development. First we investigate the properties of the eigenvectors of the Floquet Hamiltonian K. We

will see that the eigenvectors can all be simply generated from the ψ_α. To achieve this we employ the shift operator T_m on $\mathcal{K}$ defined by

$$T_m \mid \alpha n\rangle\rangle = \mid \alpha, n+m\rangle\rangle. \tag{6.6}$$

Now, using the fact that T_m commutes with H, we have

$$\begin{aligned} KT_m \mid \alpha n\rangle\rangle &= \left(-\mathrm{i}\tfrac{\partial}{\partial t} + H\right) \mathrm{e}^{\mathrm{i}(n+m)\omega t}\xi_\alpha \\ &= (n+m)\omega \mid \alpha, n+m\rangle\rangle + H \mid \alpha, n+m\rangle\rangle \end{aligned} \tag{6.7}$$

and

$$\begin{aligned} T_m K \mid \alpha n\rangle\rangle &= T_m \left(-\mathrm{i}\tfrac{\partial}{\partial t} + H\right) \mathrm{e}^{\mathrm{i}n\omega t}\xi_\alpha \\ &= n\omega \mid \alpha, n+m\rangle\rangle + H \mid \alpha, n+m\rangle\rangle, \end{aligned} \tag{6.8}$$

giving $KT_m = T_m K + m\omega T_m$.

This allows us to find the eigenvectors of the Floquet Hamiltonian K. We try the vectors $\psi_{\alpha m} = T_m \psi_\alpha$. Using equation (6.4), we find that

$$\begin{aligned} KT_m\psi_\alpha &= T_m K\psi_\alpha + m\omega T_m \psi_\alpha \\ &= (\epsilon_\alpha + m\omega) T_m \psi_\alpha. \end{aligned} \tag{6.9}$$

This means that each standard single-valued vector $\psi_\alpha(t) = Z(t)\phi_\alpha(0)$ is associated with a countably infinite stack of eigenvectors $\psi_{\alpha n} = T_n\psi_\alpha$ whose eigenvalues $\epsilon_{\alpha n}$ differ from ϵ_α by an integral multiple of ω. As vectors in $\mathcal{H}$, we have $\psi_{\alpha n} = \exp\{in\omega t\}\psi_\alpha$. We write $\psi_{\alpha 0}$ and $\epsilon_{\alpha 0}$ for ψ_α and ϵ_α for notational consistency. Note that, for a given α, the vectors $\psi_{\alpha n}(t)$ in $\mathcal{H}$ are linearly dependent at each time t, whereas the $\psi_{\alpha n}$ are linearly independent as vectors in $\mathcal{K}$.

We still have to show that this procedure exhausts the set of eigenvectors. To see why this is so, let ψ be an arbitrary eigenvector of K with eigenvalue ϵ. Further, put $\phi(t) = \exp\{-\mathrm{i}\epsilon t\}\psi(t)$. Then

$$\begin{aligned} \mathrm{i}\dot{\phi} &= \epsilon \mathrm{e}^{-\mathrm{i}\epsilon t}\psi + \mathrm{i}\mathrm{e}^{-\mathrm{i}\epsilon t}\dot{\psi} \\ &= \mathrm{e}^{-\mathrm{i}\epsilon t}\left(K + \mathrm{i}\tfrac{\partial}{\partial t}\right)\psi \\ &= \mathrm{e}^{-\mathrm{i}\epsilon t} H\psi \\ &= H\phi. \end{aligned} \tag{6.10}$$

Hence ϕ is a solution of the time-dependent Schrödinger equation. However, as ψ must be a single-valued vector (as it is an element of the Hilbert space $\mathcal{K}$), $\psi(\tilde{t}) = \exp\{i\epsilon\tilde{t}\}\phi(0)$ and so $\psi(0)$ is a cyclic initial state with overall phase $\chi = \epsilon\tilde{t}$. Now let ψ_α be the corresponding standard single-valued vector $Z\phi(0)$. Thus, as the final state must be the same whether we use ψ or ψ_α, we must have $\chi = \chi_\alpha - 2n\pi$ for some integral n. Hence $\epsilon = \epsilon_\alpha - n\omega$. Finally,

$$\begin{aligned} \phi(t) &= \mathrm{e}^{\mathrm{i}\epsilon_\alpha t}\psi_\alpha(t) \\ &= \mathrm{e}^{\mathrm{i}\epsilon t}\psi(t) \\ \Rightarrow \qquad \psi(t) &= \mathrm{e}^{\mathrm{i}(\epsilon_\alpha - \epsilon)t}\psi_\alpha \\ &= \mathrm{e}^{\mathrm{i}n\omega t}\psi_\alpha. \end{aligned} \tag{6.11}$$

But this is just $\phi_{\alpha n} = T_m\phi_\alpha$. Hence all of the eigenvectors of K are accessible from the standard set ϕ_α by the use of T_m.

The quasi-energy states have several other useful properties. For example, they can be shown to satisfy such relations as the variational principle and the Hellmann-Feynman theorem [Chu 1989]. The only other result we need concerns the normalisation of the $\psi_{\alpha n}$. In general, if the vector ψ is normalised in $\mathcal{K}$ then there is no guarantee that the corresponding vector $\psi(t)$ must be normalised in $\mathcal{H}$ at all times t. However we need the normalisation of the single-valued vector in the proof that the Berry phase is given by equation (3.8). We find that the problem is removed by the condition that $T_m\psi$ must be an eigenvector of K whenever ψ is. Let $\psi = \sum_{\alpha n} a_{\alpha n} \mid \alpha n\rangle\rangle$ be an arbitrary normalised eigenvector of K. Then

$$\begin{aligned} 1 &= \langle\langle\psi \mid \psi\rangle\rangle \\ &= \sum_{\alpha n} |a_{\alpha n}|^2. \end{aligned} \tag{6.12}$$

Further, let $\psi' = T_{-m}\psi$ for some non-zero integer m. Then ψ' is also an eigenvector of K, but with different eigenvalue. Hence ψ and ψ' must be orthogonal in $\mathcal{K}$, giving

$$0 = \langle\langle\psi' \mid \psi\rangle\rangle$$

$$= \sum_{\alpha n;\alpha' n'} \overline{a}_{\alpha' n'} a_{\alpha n} \langle\langle \alpha' n' - m \mid \alpha n \rangle\rangle$$
$$= \sum_{\alpha n} \overline{a}_{\alpha n} a_{\alpha, n+m}. \tag{6.13}$$

Combining these two results, we have that $\sum_{\alpha n} \overline{a}_{\alpha n} a_{\alpha,n+m} = \delta_{m0}$. Now, as a vector in $\mathcal{H}$, we have $\psi(t) = \sum_\alpha (\sum_n a_{\alpha n} \exp\{in\omega t\}) \mid \alpha\rangle$. Using equations (6.12) and (6.13), we can now check that $\psi(t)$ is in fact normalised in $\mathcal{H}$. We have

$$\begin{aligned}
\langle \psi(t) \mid \psi(t) \rangle &= \sum_\alpha \Big| \sum_n a_{\alpha n} \mathrm{e}^{\mathrm{i}n\omega t} \Big|^2 \\
&= \sum_\alpha \sum_{nk} \overline{a}_{\alpha n} a_{\alpha k} \mathrm{e}^{\mathrm{i}(k-n)\omega t} \\
&= \sum_{\alpha m} \sum_n \overline{a}_{\alpha n} a_{\alpha, n+m} \quad \mathrm{e}^{\mathrm{i}m\omega t} \\
&= \sum_{\alpha m} \delta_{m0} \mathrm{e}^{\mathrm{i}m\omega t} \\
&= 1.
\end{aligned} \tag{6.14}$$

Hence, $\psi(t)$ is normalised as a vector in $\mathcal{H}$ as required.

We are now in a position to be able to calculate the Berry phases. The procedure is as follows. First we find the eigenvectors $\psi_{\alpha n}$ of K. The label n is chosen so that $\psi_{\alpha 0}$ has eigenvalue $\epsilon_{\alpha 0}$ in the half-open interval $[0, \omega)$. These are the standard vectors ψ_α. We then need merely apply equation (3.8). Note that in most cases we could use any of the $\psi_{\alpha n}$, the exception being in cases of quasi-degeneracy. In these cases, using the $\psi_{\alpha 0}$ means that any quasi-degenerate cyclic initial states will have single-valued vectors that are degenerate as eigenvectors of K. Thus, as in section 5.2, using the $\psi_{\alpha 0}$ means that we must catch all of the cyclic initial states.

We can calculate the Berry phases explicitly if we expand $\psi_{\alpha 0}$ in the basis $\{| \alpha n \rangle\rangle\}$: $\psi_{\alpha 0} = \sum_{\alpha' n} a_{\alpha' n} \mid \alpha' n \rangle\rangle$. Then, as $\psi_{\alpha 0}$ is a single-valued vector, direct substitution into equation (3.8) gives

$$\begin{aligned}
\gamma_\alpha &= \mathrm{i} \int_0^{\tilde{t}} \langle \psi_\alpha \mid \dot{\psi}_\alpha \rangle \, \mathrm{d}t \\
&= \mathrm{i}\tilde{t} \langle\langle \psi_\alpha \mid \dot{\psi}_\alpha \rangle\rangle.
\end{aligned} \tag{6.15}$$

Now,

$$\begin{aligned} \mathrm{i}\dot{\psi}_\alpha &= \mathrm{i}\tfrac{\partial}{\partial t}\sum_{\alpha' n} a_{\alpha' n} \mid \alpha' n\rangle\!\rangle \\ &= -\sum_{\alpha' n} n\omega a_{\alpha' n} \mathrm{e}^{\mathrm{i}n\omega t}\xi_{\alpha'} \\ &= -\sum_{\alpha' n} n\omega a_{\alpha' n} \mid \alpha' n\rangle\!\rangle. \end{aligned} \tag{6.16}$$

Thus, as $\tilde{t} = 2\pi/\omega$,

$$\begin{aligned} \gamma_\alpha &= -\tilde{t}\omega \sum_{\alpha' n;\beta m} n\bar{a}_{\beta m} a_{\alpha' n} \langle\!\langle \beta m \mid \alpha' n\rangle\!\rangle \\ &= -2\pi \sum_{\alpha' n} n|a_{\alpha' n}|^2. \end{aligned} \tag{6.17}$$

In summary, the quasi-energy states give the single-valued vectors $Z(t)\phi(0)$ and so the Berry phases. Further, the evolution operator need not be evaluated, as all we need are the quasi-energy states. These are merely the eigenvectors of the Floquet Hamiltonian K, an operator acting on the direct product Hilbert space $\mathcal{K} = \mathcal{T} \otimes \mathcal{H}$. In the next section I will reformulate the results in matrix language. This greatly facilitates that calculation of the quasi-energy states and allows the Fourier decomposition of the Hamiltonian to be efficiently utilised.

6.2 Matrix formulation

The theory of the last section enables one to find the cyclic initial states and Berry phases from the eigenvectors of the Floquet Hamiltonian K. However, the Floquet Hamiltonian in the form (6.5) is somewhat intangible. To rectify this we write K as a matrix in the basis $\{|\, \alpha n\rangle\rangle\}$. This involves the Fourier decomposition of the Hamiltonian H and reproduces the results of Shirley [1965].

We have

$$\begin{aligned} K \mid \beta m\rangle\rangle &= (-\mathrm{i}\tfrac{\partial}{\partial t} + H)\, \mathrm{e}^{\mathrm{i}m\omega t}\xi_\beta \\ &= m\omega \mathrm{e}^{\mathrm{i}m\omega t}\xi_\beta + \mathrm{e}^{\mathrm{i}m\omega t} H\xi_\beta \\ &= (m\omega + H) \mid \beta m\rangle\rangle \\ \Rightarrow \qquad \langle\langle \alpha n \mid K \mid \beta m\rangle\rangle &= m\omega\delta_{\alpha\beta}\delta_{nm} + \langle\langle \alpha n \mid H \mid \beta m\rangle\rangle. \end{aligned} \tag{6.18}$$

Now the Hamiltonian H has Fourier decomposition

$$H(t) = \sum_n H^{[n]} \mathrm{e}^{\mathrm{i}n\omega t}, \tag{6.19}$$

where

$$H^{[n]} = \frac{1}{\tilde{t}} \int_0^{\tilde{t}} H(t) \mathrm{e}^{-\mathrm{i}n\omega t}\, \mathrm{d}t. \tag{6.20}$$

This means that

$$\begin{aligned} \langle\langle \alpha n \mid H \mid \beta m\rangle\rangle &= \langle \alpha \mid \frac{1}{\tilde{t}} \int_0^{\tilde{t}} H(t) \mathrm{e}^{-\mathrm{i}(n-m)\omega t}\, \mathrm{d}t \mid \beta\rangle \\ &= H^{[n-m]}_{\alpha\beta}, \end{aligned} \tag{6.21}$$

where the $H^{[n-m]}_{\alpha\beta}$ are the matrix elements of the $(n-m)^{\text{th}}$ Fourier component of H. Substituting this into equation (6.18) we find that K has the matrix elements

$$\langle\langle \alpha n \mid K \mid \beta m\rangle\rangle = H^{[n-m]}_{\alpha\beta} + n\omega\delta_{\alpha\beta}\delta_{nm}. \tag{6.22}$$

This is the same representation as is used in Shirley [1965]. It is instructive to discuss his derivation, as it further cements the relationship between the

Fourier theory of this chapter and the operator decomposition approach of section 5.1. Shirley solved the time-dependent Schrödinger equation Fourier component by Fourier component. The most obvious way to do this would be to use the operator Z in the decomposition $U = Z\exp\{\mathrm{i}Mt\}$. As Z is $\tilde{t}$-periodic, it should be possible to evaluate its Fourier components directly from those of the Hamiltonian. However, this is not the best approach. This is because the operator M is not diagonal in the basis ξ_α in which we are working, greatly complicating the algebra. The solution is to use a different fundamental operator.

We proceed as follows. Given the evolution operator U, any other fundamental operator F is of the form $F = UX$, where X is a constant unitary operator. This is easily proved by analogy with the proof of equation (5.6). Now $U = Z\exp\{\mathrm{i}Mt\}$. Therefore

$$\begin{aligned} F &= Z\mathrm{e}^{\mathrm{i}Mt}X \\ &= P\mathrm{e}^{\mathrm{i}Qt}, \end{aligned} \tag{6.23}$$

where

$$P = ZX, \tag{6.24}$$

$$Q = X^*MX. \tag{6.25}$$

Now we want Q to be diagonal in our chosen basis ξ_α, which requires Q to be diagonalisable. Note that this limitation on Shirley's analysis is not present in the analysis of the previous section. We assume for the moment that a complete set of cyclic initial states does exist, so that M is diagonalisable. As Q is diagonal we write $Q \mid \alpha\rangle = -\epsilon_\alpha \mid \alpha\rangle$.

We are now in a position to solve the time-dependent Schrödinger equation $\mathrm{i}\dot{F} = HF$ Fourier component by Fourier component. Substituting $F = P\exp\{\mathrm{i}Qt\}$ and using the fact that $P = \sum_n P^{[n]}\exp\{\mathrm{i}n\omega t\}$, as P is $\tilde{t}$-periodic, gives

$$\mathrm{i}\dot{P} = HP + PQ$$

$$\Rightarrow \quad \sum_n -n\omega P^{[n]}\mathrm{e}^{\mathrm{i}n\omega t} = \sum_{nm} H^{[n-m]}P^{[m]}\mathrm{e}^{\mathrm{i}n\omega t} + \sum_n P^{[n]}Q\mathrm{e}^{\mathrm{i}n\omega t}$$

$$\Rightarrow \qquad -n\omega P^{[n]} = \sum_m H^{[n-m]} P^{[m]} + P^{[n]} Q$$

$$\Rightarrow \qquad \epsilon_\beta P^{[n]}_{\alpha\beta} = \sum_{\gamma m} \left(H^{[n-m]}_{\alpha\gamma} + n\omega \delta_{\alpha\gamma} \delta_{nm} \right) P^{[m]}_{\gamma\beta}. \tag{6.26}$$

But this is just the condition that ϵ_α be an eigenvalue of the Floquet Hamiltonian H. Hence the Fourier formalism of the previous section is intimately linked to the operator decomposition formalism of section 5.1.

This formalism provides an easy way of solving the semi-classical Jaynes-Cummings model [Moore 1990a]. For a more general survey of its application to two-level problems with sinusoidal Hamiltonians, see Dion and Hirschfelder [1976]. The Hamiltonian is

$$H(t) = \begin{bmatrix} \frac{\omega}{2} & k e^{-i\omega t} \\ k e^{i\omega t} & -\frac{\omega}{2} \end{bmatrix}. \tag{6.27}$$

We denote the basis in which H is written as $\{\xi_\pm\}$. By inspection, the Fourier components of H are given by

$$H^{[1]} = \begin{bmatrix} 0 & 0 \\ k & 0 \end{bmatrix}, \tag{6.28}$$

$$H^{[0]} = \begin{bmatrix} \frac{\omega}{2} & 0 \\ 0 & -\frac{\omega}{2} \end{bmatrix}, \tag{6.29}$$

$$H^{[-1]} = \begin{bmatrix} 0 & k \\ 0 & 0 \end{bmatrix}, \tag{6.30}$$

with all other components vanishing. Now, as $\langle\langle \alpha n \mid K \mid \beta m \rangle\rangle = H^{[n-m]}_{\alpha\beta} + n\omega\delta_{\alpha\beta}\delta_{nm}$, we can see that n and m can differ by at most unity. Thus K must be block tri-diagonal in the ordered basis $\{\ldots, |+1\rangle\rangle, |-1\rangle\rangle, |+0\rangle\rangle, \ldots\}$:

$$K = \begin{bmatrix} \ddots & \ddots & \ddots & & & 0 \\ & Z_1 & X_1 & Y_1 & & \\ & & Z_0 & X_0 & Y_0 & \\ 0 & & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{6.31}$$

where the blocks are all 2×2 matrices. Now $[Z_n]_{\alpha\beta} = \langle\langle \alpha n \mid K \mid \beta n + 1 \rangle\rangle = H^{[-1]}_{\alpha\beta}$ so that

$$Z_n = \begin{bmatrix} 0 & k \\ 0 & 0 \end{bmatrix}. \tag{6.32}$$

Also $[Y_n]_{\alpha\beta} = \langle\langle \alpha n \mid K \mid \beta n - 1 \rangle\rangle = H^{[1]}_{\alpha\beta}$. Hence

$$Y_n = \begin{bmatrix} 0 & 0 \\ k & 0 \end{bmatrix}. \tag{6.33}$$

Finally $[X_n]_{\alpha\beta} = \langle\langle \alpha n \mid K \mid \beta n \rangle\rangle = H^{[0]}_{\alpha\beta} + n\omega\delta_{\alpha\beta}$ giving

$$X_n = \begin{bmatrix} n\omega + \frac{\omega}{2} & 0 \\ 0 & n\omega - \frac{\omega}{2} \end{bmatrix}. \tag{6.34}$$

Substituting into (6.31), we find that

$$K = \begin{array}{c} \\ 1+ \\ 1- \\ 0+ \\ 0- \\ \\ \end{array} \begin{array}{c} \begin{array}{cccccccc} & & 1+ & 1- & 0+ & 0- & & \end{array} \\ \begin{bmatrix} \ddots & \ddots & \ddots & & & & & 0 \\ & k & \frac{3\omega}{2} & 0 & & & & \\ & & 0 & \frac{\omega}{2} & k & & & \\ & & & k & \frac{\omega}{2} & 0 & & \\ & & & & 0 & -\frac{\omega}{2} & k & \\ 0 & & & & & \ddots & \ddots & \ddots \end{bmatrix} \end{array} \tag{6.35}$$

Thus the Floquet Hamiltonian is block diagonal with typical block

$$K_n = \begin{bmatrix} (n + \frac{1}{2})\omega & k \\ k & (n + \frac{1}{2})\omega \end{bmatrix} \tag{6.36}$$

in the basis $\{| -, n+1\rangle\rangle, | +, n\rangle\rangle\}$.

Hence, to find the eigenvectors of K (the quasi-energy states) we need merely find the eigenvectors of the typical block. In fact, if we ignore quasi-degeneracy, any block would do, but not much extra labour is needed for the general case. By direct substitution it is easy to show that H_n has eigenvectors

$$\psi_{\pm n} = \sqrt{\tfrac{1}{2}} \begin{bmatrix} \pm 1 \\ 1 \end{bmatrix}, \tag{6.37}$$

with eigenvalues

$$\epsilon_{\alpha n} = (n + \tfrac{1}{2})\omega \pm k. \tag{6.38}$$

Now, noting that the vector $\psi_{\pm n}$ is written in the basis $\{|-,n+1\rangle\rangle, |+,n\rangle\rangle\}$, we have that

$$\begin{aligned}\psi_{\alpha n} &= \pm\sqrt{\tfrac{1}{2}}\,|-,n+1\rangle\rangle + \sqrt{\tfrac{1}{2}}\,|+,n\rangle\rangle \\ &= \pm\sqrt{\tfrac{1}{2}}\mathrm{e}^{\mathrm{i}(n+1)\omega t}\xi_- + \sqrt{\tfrac{1}{2}}\mathrm{e}^{\mathrm{i}n\omega t}\xi_+. \end{aligned} \tag{6.39}$$

Thus, interpreting $\psi_{\pm,n}(t)$ as a single-valued vector, the cyclic initial states are given by

$$\phi_\pm(0) = \pm\sqrt{\tfrac{1}{2}}\xi_- + \sqrt{\tfrac{1}{2}}\xi_+, \tag{6.40}$$

with Berry phases, from equation (6.17),

$$\begin{aligned}\gamma_\pm &= -2\pi \sum_{\pm' n} n|a_{\pm' n}|^2 \\ &= -2\pi\left(\tfrac{1}{2}(n+1) + \tfrac{1}{2}n\right) \\ &= \pi \qquad (\mathrm{mod}\ 2\pi), \end{aligned} \tag{6.41}$$

in agreement with equation (5.21).

For more difficult Hamiltonians, an exact solution may not be possible. However, even for these systems the Fourier method has an advantage over the more direct algorithms. This is because here we can use the powerful methods of time-independent perturbation theory, instead of having to use the weaker time-dependent theory.

Chapter Seven

Other formalisms

In the previous two chapters I have used two methods to calculate Berry phases. The first involves decomposing the evolution operator into the product form $U = Z\exp\{\mathrm{i}Mt\}$. Here Z is $\tilde{t}$-periodic and unitary, while M is constant and self-adjoint with spectrum in $[0, 2\pi/\tilde{t})$. The second method converts the problem into an equivalent time-independent one using the Floquet Hamiltonian. In this chapter I describe two other methods. While I have not been directly involved with either of them, I summarise them here to place my work in context within the rest of the field.

In section 7.1, I analyse the first of these approaches. This uses the geometrical structure of the Hilbert space to display the Berry phase in terms of the holonomy of a suitable fibre bundle (see section A.2). In this way the geometric nature of the Berry phase is made plain. Further, we find that the Berry phase depends only on the path followed by the system in projective Hilbert space, not on the details of the Hamiltonian. This point can also be made using our original single-valued vector approach. As the determination of the single-valued vectors only requires the relevant paths in projective Hilbert space, the Berry phases do not depend on the other details of the Hamiltonian. The geometric method was first discussed by Simon [1983] in the adiabatic context, and was generalised to the non-adiabatic case by Aharonov and Anandan [1987].

In section 7.2, the Lie algebraic approach is discussed. This method can be applied to systems whose Hamiltonians are members of some Lie algebra. The evolving states can then be described in terms of the generalised coherent states (see section B.3). This method was first used by Brihaye *et al.* [1990], following the

work of Giavarini and Onofri [1989]. Similar ideas are used in section 8.2, where I discuss the existence of cyclic initial states for the forced harmonic oscillator.

7.1 Geometric approaches

Up until now, the Berry phases have been calculated using single-valued vectors. To get a single-valued vector $\psi(t)$ from the evolving state $\phi(t)$ we merely rephase ϕ in such a (time-dependent) way that $\psi(\tilde{t}) = \psi(0)$. However, we can also calculate the Berry phases using a different rephasing approach. Let $\zeta(t) = \exp\{\mathrm{i}\theta(t)\}\phi(t)$ where $\theta(t) = \mathrm{i}\int_0^t \langle\phi \mid \dot{\phi}\rangle \,\mathrm{d}t'$. Then

$$\langle\zeta \mid \dot{\zeta}\rangle = \mathrm{i}\dot{\theta} + \langle\phi \mid \dot{\phi}\rangle = 0. \tag{7.1}$$

In fact, assuming that $\zeta(0) = \phi(0)$, ζ is the only vector following ϕ with this property [Anandan and Stodolsky 1987].

Now assume that $\phi(0)$ is a cyclic initial state with overall phase χ. Then, using the fact that $H\phi = \mathrm{i}\dot{\phi}$, the corresponding Berry phase is given by

$$\begin{aligned}\gamma &= \chi - \delta \\ &= \chi + \mathrm{i}\int_0^{\tilde{t}} \langle\phi \mid \dot{\phi}\rangle \,\mathrm{d}t \\ &= \chi + \theta(\tilde{t}).\end{aligned} \tag{7.2}$$

But

$$\begin{aligned}\zeta(\tilde{t}) &= \mathrm{e}^{\mathrm{i}\theta(\tilde{t})}\phi(\tilde{t}) \\ &= \mathrm{e}^{\mathrm{i}(\chi+\theta(t))}\psi(0).\end{aligned} \tag{7.3}$$

Hence the Berry phase is just the phase picked up by the vector ζ as it follows the evolving state ϕ. This is the basis of the geometric method.

To proceed we need some differential geometry. More detail is given in section A.2. Imagine that the Hilbert space of interest is finite dimensional. That is, $\mathcal{H} = \mathbb{C}^{n+1}$. Then the normalised states are members of the sphere S^{2n+1}. If

the Hilbert space is taken to be infinite dimensional, then the relevant space is the injective limit of odd spheres [Boya and Sudarshan 1990]. Now, as there is an arbitrary phase in quantum mechanics, the physical states are the equivalence classes of elements of S^{2n+1} that are equal up to a phase. This is the projective Hilbert space $\mathcal{P}$.

These geometric structures are related by the notion of a fibre bundle. Each point in the set S^{2n+1} projects onto a point in $\mathcal{P}$, the equivalence class to which it belongs. Further, if two points in S^{2n+1} project onto the same point of $\mathcal{P}$ they must be equal up to a phase. Thus the set of points of S^{2n+1} which project onto a single given point of $\mathcal{P}$ is isomorphic to the group of phases $U(1)$. In mathematical language, the set of normalised states is a fibre bundle over the projective Hilbert space with structure group $U(1)$.

Now as I mentioned earlier this chapter, the Berry phase is completely determined by the path $\mathcal{C}$ followed by the system in projective Hilbert space. Of course this path does not determine the path followed by the system in S^{2n+1}, as there is a time-dependent phase ambiguity. To do a calculation in $\mathcal{H}$ we need to choose one of the infinity of paths in S^{2n+1} that projects onto $\mathcal{C}$. Such a choice is called a connection.

We have at our disposal three possible choices of connection; the state vector $\phi(t)$ itself, the corresponding single-valued vector $\psi(t)$ or the vector $\zeta(t)$ satisfying (7.1). The state vector is not a good choice, as it obviously depends on the Hamiltonian, not just the path followed by the system in projective Hilbert space. Further, the single-valued vector is not unique. This is because if $\psi(t)$ is a single-valued vector, then so is $\exp\{i\alpha(t)\}\psi(t)$ for any α with $\alpha(\tilde{t}) = \alpha(0) = 0$. While we could take the single-valued vector $Z(t)\phi(0)$ used in section 5.1, this choice is not intuitively better than any other. In contrast, the vector $\zeta(t)$ is unique, making it a logical choice of connection.

That this is indeed the best choice follows from the following two observations. The condition $\langle \zeta \mid \dot{\zeta} \rangle = 0$ is precisely the requirement for the natural connection induced by the inner product of the Hilbert space [Bohm *et al.* 1990]. Further,

the Berry phase is just the phase change suffered by ζ as it follows the closed path in $\mathcal{P}$. This is called the holonomy of the connection.

In other words, the Berry phase is just the holonomy of the natural connection. This was first noted by Simon [1983] for the adiabatic case, his work being extended to non-adiabatic evolution by Aharonov and Anandan [1987]. This motivates the description of the Berry phase as a geometrical phase. It is determined by the geometry of the path $\mathcal{C}$ followed by the system in projective Hilbert space.

Up until now, the Berry phase has been calculated using the elements of $\mathcal{H}$, the state vectors. But, as the Berry phase only depends on the path $\mathcal{C}$, we should be able to express it in terms of a coordinatisation of the projective Hilbert space $\mathcal{P}$. Now, as the Hilbert space is taken to be $\mathbb{C}^{n+1}$, a state in $\mathcal{H}$ can be written in terms of $n+1$ complex amplitudes:

$$|\,\phi\rangle = |\,X^0, X^1, \ldots, X^n\rangle. \tag{7.4}$$

For simplicity, we assume that $X^0(t)$ is non-zero throughout the evolution. This means that we can give the projective Hilbert space the complex coordinates

$$w^i = \frac{X^i}{X^0}, \tag{7.5}$$

where $i = 1, \ldots, n$. Page [1987] then shows that the Berry phase is given by

$$\gamma = \oint A, \tag{7.6}$$

where the one-form A is

$$A = \frac{\mathrm{i}}{2} \frac{\overline{w}_i \, \mathrm{d}w^i - w_i \, \mathrm{d}\overline{w}^i}{1 + \overline{w}_k w^k}. \tag{7.7}$$

Hence the Berry phase can be written in terms of a coordinatisation of the projective Hilbert space. For instance, consider the semi-classical Jaynes-Cummings model with zero detuning:

$$H(t) = \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix} \tag{7.8}$$

By direct substitution, one can verify that the general initial state

$$\phi(0) = \sqrt{\tfrac{1}{2}}a_+ \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \sqrt{\tfrac{1}{2}}a_- \begin{bmatrix} -1 \\ 1 \end{bmatrix} \tag{7.9}$$

evolves into

$$\phi(t) = \sqrt{\tfrac{1}{2}}a_+ \mathrm{e}^{-\mathrm{i}kt} \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t/2} \\ \mathrm{e}^{\mathrm{i}\omega t/2} \end{bmatrix} + \sqrt{\tfrac{1}{2}}a_- \mathrm{e}^{\mathrm{i}kt} \begin{bmatrix} -\mathrm{e}^{-\mathrm{i}\omega t/2} \\ \mathrm{e}^{\mathrm{i}\omega t/2} \end{bmatrix}. \tag{7.10}$$

Hence the cyclic initial states are found by taking either $a_+ = 1$ or $a_- = 1$, with the other coefficient being zero.

In terms of Page's coordinatisation, we have

$$X_+ = \pm\sqrt{\tfrac{1}{2}}\mathrm{e}^{-\mathrm{i}\omega t/2}\mathrm{e}^{\mp \mathrm{i}kt}, \tag{7.11}$$

$$X_- = \sqrt{\tfrac{1}{2}}\mathrm{e}^{\mathrm{i}\omega t/2}\mathrm{e}^{\mp \mathrm{i}kt}. \tag{7.12}$$

As the Hilbert space is two-dimensional, the projective Hilbert space is one-dimensional. Its single coordinate λ is given by

$$\lambda = \frac{X_+}{X_-} = \pm\mathrm{e}^{-\mathrm{i}\omega t}. \tag{7.13}$$

Hence the one form A is given by

$$\begin{aligned} A &= \frac{\mathrm{i}}{2}\frac{\overline{\lambda}\,\mathrm{d}\lambda - \lambda\,\mathrm{d}\overline{\lambda}}{1 + \overline{\lambda}\lambda} \\ &= \tfrac{\omega}{2}\,\mathrm{d}t. \end{aligned} \tag{7.14}$$

Substituting into equation (7.6), the Berry phase is then given by

$$\gamma = \int_0^{2\pi/\omega} \tfrac{\omega}{2}\,\mathrm{d}t = \pi, \tag{7.15}$$

in agreement with the other approaches.

The Berry phase can also be expressed using Fermi-Walker parallel transport. We specialise to the adiabatic case for simplicity. Consider an adiabatic Hamiltonian $H = \mathbf{R} \cdot \boldsymbol{\sigma}$, where the vector $\mathbf{R}$ follows the space curve γ. We describe γ

in terms of the length s, curvature k and torsion τ. The tangent vector, principal normal and binormal are then given by the Frenet-Serret formulae [Dandoloff 1989]

$$\dot{\mathbf{t}} = k\mathbf{n}, \qquad \dot{\mathbf{n}} = -k\mathbf{t} + \tau\mathbf{b} \qquad \text{and} \qquad \dot{\mathbf{b}} = -\tau\mathbf{n} \tag{7.16}$$

respectively. Now, as H is assumed to be adiabatic, the relevant vectors are suitably phased eigenvectors. Further, the requirement (7.1) means that a frame parallel transported with $\mathbf{t}$ has angular momentum $\mathbf{\Omega} = \mathbf{t} \times \dot{\mathbf{t}} = k\mathbf{b}$. This frame is just the Fermi-Walker transported one.

In contrast, the triad $\mathbf{t}, \mathbf{b}, \mathbf{n}$ has angular momentum $\mathbf{\Omega}' = \mathbf{n} \times \dot{\mathbf{n}}$. One can show that the Berry phase is just the integral of the difference between these two angular momenta [Dandoloff 1989]:

$$\gamma = \int (\mathbf{\Omega}' - \mathbf{\Omega}) \cdot \mathbf{t}\, ds. \tag{7.17}$$

Hence the Berry phase is related to the twisting of the Fermi-Walker transported frame around the triad $\mathbf{t}, \mathbf{b}, \mathbf{n}$, again pointing to its geometric nature. This approach has been applied to the classical continuous antiferromagnetic Heisenberg spin chain [Balakrishnan *et al.* 1990].

Finally, we note that the dynamical phase also has a geometric nature. This can be seen by treating the Schrödinger formulation of quantum mechanics as a classical field theory [Ralston 1989].

7.2 Lie algebraic approaches

Having discussed geometric methods for the calculation of non-adiabatic Berry phases, I now turn to the Lie algebraic approach. If the Hamiltonian of interest is a member of some Lie algebra, then the evolution operator must be an element of the corresponding Lie group. This means that the evolving state is just a generalised coherent state (see section B.3). The Berry phases can then be found in terms of the Cartan forms of the algebra. The development given here is based on the work of Brihaye *et al.* [1990]. The special case of Hamiltonians of the form $H(t) = V(t)H(0)V^*(t)$, with V unitary, was first considered by Giavarini and Onofri [1989].

Consider a time-dependent Hamiltonian $H(t)$ that can be written as a linear combination of the basis elements X_j of some Lie algebra:

$$H(t) = \sum_{j=1}^{n} a_j(t) X_j. \tag{7.18}$$

Further, let the corresponding Lie group G have unitary representation $T(g)$ on the Hilbert space $\mathcal{H}$. Now the evolution operator $U(t)$ can be written as the time-ordered integral

$$U(t) = \mathcal{T}\exp\{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'\}, \tag{7.19}$$

and so is a member of the representation T. That is, there exists an element $g(t)$ of G such that

$$U(t) = T(g(t)). \tag{7.20}$$

This fact is the basis of the Lie algebraic method.

We can display explicitly the evolution operator as an element of T in many different ways. The simplest such characterisations involve exponential decompositions. For example, Wei and Norman [1963] show that $U(t)$ can locally be written in the form

$$U(t) = \prod_{j=1}^{n} \exp\{\alpha_j(t) X_j\}. \tag{7.21}$$

As this is a product of elements of G, so is the evolution operator. Note that this description is global if G is solvable, but is not so in general. Further, Wilcox [1967] shows that the evolution operator can also be locally expressed as

$$U(t) = \exp\{\sum_{j=1}^{n} \beta_j(t) X_j\}. \tag{7.22}$$

Then, as $\sum_{j=1}^{n} \beta_j(t) X_j$ is in the Lie algebra of G, $U(t)$ is manifestly a group element.

As an example of the forms (7.21) and (7.22), consider the Hamiltonian

$$H(t) = \tfrac{1}{2}\left(a(t)p^2 + b(t)q^2\right). \tag{7.23}$$

Then we may take

$$X_1 = \tfrac{1}{2}q^2, \qquad X_2 = \tfrac{1}{2}(qp + pq) \qquad \text{and} \qquad X_3 = \tfrac{1}{2}p^2. \tag{7.24}$$

Now, for $u = p, q$, solve the coupled c-number equations

$$\dot{P}_u = -bQ_u \qquad \text{and} \qquad \dot{Q}_u = aP_u, \tag{7.25}$$

with the initial conditions

$$P_p(0) = Q_q(0) = 1 \qquad \text{and} \qquad P_q(0) = Q_p(0) = 0. \tag{7.26}$$

Then Pechukas and Light [1966] show that the decomposition (7.21) is given by

$$\alpha_1 = \mathrm{i}\frac{P_q}{Q_q}, \qquad \alpha_2 = -\tfrac{\mathrm{i}}{2}\ln Q_q \qquad \text{and} \qquad \alpha_3 = -\tfrac{\mathrm{i}}{2}\frac{Q_p}{Q_q}. \tag{7.27}$$

Further, Fernández [1987] shows that the decomposition (7.22) is given by the solution of the system of linear equations

$$P_p = \cos\omega - \beta_2\frac{\sin\omega}{\omega}, \tag{7.28}$$

$$P_q = -\beta_1\frac{\sin\omega}{\omega}, \tag{7.29}$$

$$Q_q = \cos\omega + \beta_2\frac{\sin\omega}{\omega}, \tag{7.30}$$

$$Q_p = \beta_3\frac{\sin\omega}{\omega}, \tag{7.31}$$

where $\omega = \beta_1\beta_3 - \beta_2^2$.

We are now in a position to express a general evolving vector as a generalised coherent state. Fix an initial state ϕ_0. We need the isotropy subspace S of G corresponding to ϕ_0. This is just the set of elements h of G for which $T(h)\phi_0 = \exp\{\mathrm{i}\alpha(h)\}\phi_0$. Then we may write any $g \in G$ in the form

$$g = \zeta h, \tag{7.32}$$

where $h \in S$ and ζ represents an equivalence class in $X = G/S$. Thus the initial state ϕ_0 evolves into

$$\begin{aligned}\phi(t) &= U(t)\phi_0 \\ &= \mathrm{e}^{\mathrm{i}\alpha(h(t))}T(\zeta(t))\phi_0.\end{aligned} \tag{7.33}$$

But $T(\zeta(t))\phi_0$ is just a generalised coherent state (see section B.3). Hence the Hamiltonian (7.18) preserves generalised coherence.

Several authors have demonstrated this coherence preservation explicitly for model Hamiltonians. For instance, the Hamiltonian

$$H(t) = \omega(t)b^*b + f(t)b^* + \overline{f}(t)b + \beta(t), \tag{7.34}$$

which is in the extended Heisenberg-Weyl algebra, was shown by Glauber [1966] to preserve standard coherent states. This Hamiltonian is treated in more detail in section 8.2. There I show that it provides a system where either a complete set of cyclic initial states exist or none do. The $SU(1,1)$ case is treated by Gerry [1985]. Systems of this type include the degenerate parametric oscillator.

Equation (7.33) can be used to provide the Berry phases. Requiring that $\zeta(\tilde{t}) = \zeta(0)$ guarantees that the initial state ϕ_0 be cyclic. Further, the vector $T(\zeta(t))\phi_0$ can then be used as a single-valued vector. Substituting into equation (3.8) then gives the Berry phase. We can also proceed algebraically. Let T_λ and T_i be the generators corresponding to S and $X = G/S$ respectively. Then the Hamiltonian may be written

$$H(t) = a^\lambda(\xi(t))T_\lambda + a^i(\xi(t))T_i, \tag{7.35}$$

for some parameter $\xi(t)$. Note that the summation convention has been used. We introduce the Cartan forms $\omega_i^\lambda(\zeta)$ and $\eta_i^j(\zeta)$ by

$$\mathrm{i}T^*(\zeta)\partial_i T(\zeta) = \omega_i^\lambda(\zeta)T_\lambda + \eta_i^j(\zeta)T_j. \tag{7.36}$$

These forms can be used to find the element ζ in X once ξ is known [Brihaye *et al.* 1990]. We have

$$\dot{\zeta}^i\eta_i^j(\zeta) = D_\lambda^j(\zeta)a^\lambda(\xi) + D_i^j(\zeta)a^i(\xi), \tag{7.37}$$

where $D(\ldots)$ is the adjoint representation of G.

Substituting into equation (3.8), the Berry phase can then be expressed in the form

$$\gamma = \oint \left(\omega_i^\lambda(\zeta)\tau_\lambda + \eta_i^j(\zeta)\langle\phi_0 \mid T_j\phi_0\rangle\right) \mathrm{d}\zeta^i, \tag{7.38}$$

where $T_\lambda\phi_0 = \tau_\lambda\phi_0$. Note that this expression only depends on the Cartan forms on the factor space $X = G/S$. The existence of cyclic initial states is guaranteed by the existence of cyclic solutions to equation (7.37). This fact is used in section 8.2, where I discuss the existence of cyclic initial states for the forced harmonic oscillator.

As an example of this formalism, consider a classical spin in a magnetic field. The Hamiltonian $H(t) = -(\mu/j)\mathbf{J}\cdot\mathbf{B}$ can be expressed in terms of the $SU(2)$ generators in the form [Layton *et al.* 1990]

$$H(t) = \mathrm{i}(aJ_+ - \overline{a}J_- - \mathrm{i}bJ_0), \tag{7.39}$$

where $a = \mathrm{i}(\mu/2j)(B_x - \mathrm{i}B_y)$ and $b = -(\mu/j)B_z$. The isotropy subgroup for this problem is just $U(1)$, so that the coherent states are given by

$$\mid \xi\rangle = \mathrm{e}^{\xi J_+ - \overline{\xi}J_-} \mid j,m\rangle. \tag{7.40}$$

As $\langle j,m \mid J_\pm \mid j,m\rangle = 0$ we only need the Cartan form related to $S = U(1)$. This is given by [Brihaye *et al.* 1990]

$$\omega = \frac{\mathrm{i}(\xi\,\mathrm{d}\overline{\xi} - \overline{\xi}\,\mathrm{d}\xi)}{2|\xi|^2}(1 - \cos 2|\xi|). \tag{7.41}$$

Thus equation (7.38) gives

$$\gamma = im \oint \frac{1-\cos 2|\xi|}{2|\xi|^2}(\xi\, \mathrm{d}\overline{\xi} - \overline{\xi}\, \mathrm{d}\xi). \tag{7.42}$$

This can be related to the expression gained by Berry for the same problem [Berry 1984]. If the magnetic field has direction

$$\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{7.43}$$

then $\xi = -\theta\exp\{-i\phi\}/2$. Substituting into equation (7.42) then gives Berry's result. Note that the quantum group analogue of the $SU(2)$ problem has been discussed by Soni [1990].

We can also consider $SU(1,1)$ Hamiltonians such as the harmonic oscillator with time-dependent frequency [Brihaye *et al.* 1990]:

$$H(t) = \tfrac{1}{2}(p^2 + \omega^2(t)q^2). \tag{7.44}$$

If we take ϕ_0 to be an eigenvector of the initial Hamiltonian $H(0) = 2\omega(0)K_3$ with eigenvalue $E(0)$, then the isotropy subgroup S is just $U(1)$. Hence

$$G/S = \{\mathbf{n} | n_3^2 - n_1^2 - n_2^2 = 1, n_3 > 0\}. \tag{7.45}$$

The relevant coherent states are given by

$$|\,\xi\rangle = \mathrm{e}^{\xi K_+ - \overline{\xi} K_-}\phi_0, \tag{7.46}$$

where $\xi = -\tau\exp\{-i\phi\}/2$ and $\mathbf{n} = (\sinh\tau\cos\phi, \sinh\tau\sin\phi, \cosh\tau)$. The Cartan form corresponding to S is then

$$\omega = -\mathrm{i}\frac{\xi\, \mathrm{d}\overline{\xi} - \overline{\xi}\, \mathrm{d}\xi}{2|\xi|^2}(1 - \cosh 2|\xi|). \tag{7.47}$$

Hence the Berry phase is given by

$$\gamma = -\mathrm{i}E(0) \oint \frac{\xi\, \mathrm{d}\overline{\xi} - \overline{\xi}\, \mathrm{d}\xi}{2|\xi|^2}(1 - \cosh 2|\xi|). \tag{7.48}$$

The Lie algebraic approach given here can also be used to disentangle general exponential operators. That is, it can be used to convert the form $\exp\{\sum_{j=1}^{n} a_j X_j\}$ into the form $\prod_{j=1}^{n} \exp\{c_j X_j\}$. For example, consider the Lie group $SU(2)$ with generators J_+, J_- and J_0. The first exponential form is

$$S = \exp\{a_1 J_+ + a_2 J_0 + a_3 J_-\}. \tag{7.49}$$

Now let the functions $c_j(\lambda)$ satisfy the coupled set of differential equations

$$\partial_\lambda c_1 = a_1 + a_2 c_1 - a_3 c_1^2, \tag{7.50}$$

$$\partial_\lambda c_2 = a_2 - 2a_3 c_1, \tag{7.51}$$

$$\partial_\lambda c_3 = a_3 \mathrm{e}^{c_2}, \tag{7.52}$$

with $c_1(0) = c_2(0) = c_3(0) = 0$. Then the second exponential form is given by [Cheng and Fung 1988]

$$S = \exp\{c_1(1)J_+\}\exp\{c_2(1)J_0\}\exp\{c_3(1)J_-\}. \tag{7.53}$$

Cheng and Fung also treat the $SU(2) \oplus h(4)$ case [Cheng and Fung 1990].

Finally, the Lie algebraic approach is also useful in the adiabatic limit. For example, Hong-Yi and Zaidi [1988] analyse the $SU(1,1)$ adiabatic limit and Cerveró and Lejarreta [1989] discuss the $SO(2,1)$ case.

Chapter Eight

The existence of cyclic states

In the previous three chapters I have discussed methods for the calculation of Berry phases. However, while these methods are very efficient for calculating the Berry phases for specific problems, they are not well suited to providing general results on the existence of cyclic initial states. In general we must find the eigenvectors of either the monodromy operator $U(\tilde{t})$ or the Floquet Hamiltonian K before we can tell if any cyclic initial states exist. As well as being computationally time consuming, these methods are specific to the problem under study. Note that we do have two general results. In section 4.1 I showed that for adiabatically varying Hamiltonians, the instantaneous eigenvectors of the initial Hamiltonian $H(0)$ are the cyclic initial states. Further, in section 5.3 I showed that, for Hamiltonians of the form $H(t) = \exp\{-\mathrm{i}At\}H(0)\exp\{\mathrm{i}At\}$, the cyclic initial states are precisely the eigenvectors of the time-independent operator $B = H(0) - A$. Hence we know the cyclic initial states for these two examples once the Hamiltonian is known.

In this chapter I will investigate the existence of cyclic initial states in some detail. For systems with finite-dimensional Hilbert spaces, we find that the existence of a complete set of cyclic initial states can be proved by a little simple linear algebra. In section 8.1 this analysis is carried further by considering systems for which the Hamiltonian $H(t)$ commutes with some time-independent operator X at all times t. For these systems, an initial state in one of the eigenspaces of X stays in that eigenspace. Thus, assuming that the eigenspaces of X are at most finitely degenerate, the problem is reduced to a countable set of effectively finite-dimensional problems. A good example is a single electron in an octahedral environment that is rotating with constant velocity about the z axis [Moore and

Stedman 1990b]. Here the Hamiltonian commutes with L^2 and $\exp\{i\pi L_z/2\}$.

In section 8.2 I discuss the periodically forced harmonic oscillator. This system is instructive as its behaviour critically depends on the existence of a certain Fourier component in the forcing term. If this component is not present then all states are cyclic with the same overall phase. This is the ultimate example of quasi-degeneracy. However, if this component is present, then there do not exist any cyclic initial states [Moore 1990b]. The derivation of these results will be couched in the language of coherent states (see appendix B). This is because the forced harmonic oscillator can be shown to preserve coherence [Glauber 1966], allowing the evolving state to be expressed in terms of the solutions to the classical equation of motion.

Finally, in section 8.3 I discuss the application of functional analysis to this problem. This makes strong use of the operator decomposition (5.8). Although no complete characterisation of which Hamiltonians have a complete set of cyclic initial states is known, several interesting systems can be discussed. For example, the results of the previous section can be verified. This method uses the notion of bounded states, that is states which essentially stay in a bounded region of space uniformly in time [Enss and Veselić 1983]. Note that this notion is also important for the existence of periodic solutions to real systems of differential equations [Yoshizawa 1975, p164].

8.1 Reducing subspaces

Consider a system with a finite dimensional Hilbert space. Then, as the monodromy operator $U(\hat{t})$ is a finite-dimensional normal matrix, it has a complete set of eigenvectors. But these are just the cyclic initial states. Hence systems with finite-dimensional Hilbert spaces always have a complete set of cyclic initial states. However things are not as simple in infinite-dimensional Hilbert spaces, where not all normal operators are diagonalisable. For example, consider the operator $\hat{x}$ defined on the Hilbert space $L^2(\mathbb{R}, \mathrm{d}x)$. This operator is of course the most physically fundamental self-adjoint operator for the particle on the line. We note that the elements of $L^2(\mathbb{R}, \mathrm{d}x)$ are not the square integrable functions $f : \mathbb{R} \to \mathbb{R}$, but equivalence classes of such functions, where two square integrable funtions are equivalent if they agree almost everywhere (see appendix A). Let $\hat{x}$ have eigenvector $\xi(x)$ with eigenvalue x': $\hat{x}\xi(x) = x'\xi(x)$. But by definition, $\hat{x}\xi(x) = x\xi(x)$. For these two expressions to agree, $\xi(x)$ must be zero except at $x = x'$. However, this means that it is zero almost everywhere and so is the zero vector of $L^2(\mathbb{R}, \mathrm{d}x)$. Then, as x' is only an eigenvalue of $\hat{x}$ if it has a corresponding non-zero eigenvector, $\hat{x}$ does not have any eigenvalues.

One simple way of guaranteeing the existence of cyclic initial states is to show that the problem in question can be considered as a countable sum of finite-dimensional problems. The motivation for this comes from the case of a time-independent Hamiltonian H. Then, if ξ is an eigenvector of H with eigenvalue E, the initial state $\phi(0) = \xi$ evolves into $\phi(t) = \exp\{-\mathrm{i}Et\}\xi$. In other words, a state initially in the space spanned by ξ stays in that space. But this means that we can ignore the rest of the eigenvectors and treat the problem as if it had a one-dimensional Hilbert space.

For some time-dependent problems, such as the single particle in a rotating octahedral environment, a similar partition can be made. Let the system of interest have Hamiltonian $H(t)$. Further, let X be a time-independent operator that commutes with the Hamiltonian at all times. A trivial example of such an

operator is the identity operator. Now, let $\mathcal{P}$ be an eigenspace of X. Then, as $H(t)$ and X commute, there must be a basis $\{\xi_a(t)\}$ of X such that each $\xi_a(t)$ is an eigenvector of $H(t)$: $H(t)\xi_a = E_a(t)\xi_a$. Note that, if the Hamiltonian does not commute with itself at different times, the vectors $\xi_a(t)$ must be time-dependent. Now, let $\Xi = \sum_a c_a\xi_a(t)$ be an arbitrary element of $\mathcal{P}$ for some given t. Then $H(t)\Xi = \sum_a c_a E_a(t)\xi_a(t)$, which is also an element of $\mathcal{P}$. Thus X is invariant under the action of H. But this implies that if the initial state is in $\mathcal{P}$, then the evolving state stays in $\mathcal{P}$.

Thus, if $\mathcal{P}$ is finite-dimensional, the problem is reduced to an equivalent finite-dimensional one and the existence of cyclic initial states is guaranteed. I will call a Hamiltonian for which this is possible *reducible*. If there is no such operator, and so no such reducing space, then the time-dependent Hamiltonian is called irreducible. This implies that no operator commutes with the Hamiltonian at all times except for multiples of the identity. This is just Schur's second lemma [Jordan 1969, p.68]. This fact points to the relevance of group theory in the existence problem.

For example, consider a single particle in an octahedral environment that rotates about the z axis with constant velocity ω. Then the Hamiltonian is given by

$$H(t) = T + \mathrm{e}^{-\mathrm{i}\omega t L_z} V \mathrm{e}^{\mathrm{i}\omega t L_z}, \tag{8.1}$$

where the exponentials represent the rotation, T is the kinetic energy operator and V is the potential energy operator, assumed to have octahedral symmetry. We will see that the existence of cyclic states for this problem is guaranteed by the invariance properties of the Hamiltonian with respect to the octahedral group. In terms of the angular momentum operator L_z we have, using the fact that L_z and T commute,

$$H(t) = \mathrm{e}^{-\mathrm{i}\omega t L_z} H(0) \mathrm{e}^{\mathrm{i}\omega t L_z}. \tag{8.2}$$

Note that H is of the form (5.45). Thus we could use Salzman's decomposition,

giving the cyclic initial states as eigenvectors of the time-independent operator $B = H(0) - \omega L_z$. However it is also a good example of a reducible Hamiltonian.

As V has octahedral symmetry, the Hamiltonian $H(t)$ commutes with L^2 at all times t. Hence we may restrict our attention to the eigenspace $\{|\, ll\rangle, |\, l, l-1\rangle \ldots, |\, l-l\rangle\}$ for given fixed l. However we can also go further. An arbitrary rotation $R_z(\theta)$ about the z axis commutes with both the kinetic energy T and the operators $\exp\{\pm i\omega t L_z\}$. Hence, if it also commutes with the potential V, it will commute with the Hamiltonian $H(t)$. Now V has octahedral symmetry, so it must commute with the operations of the group $\mathrm{O_h}$. In particular it must commute with a quarter rotation about the z axis, that is with $\exp\{-i\pi L_z/2\}$. For convenience let us consider the vectors with $l = 2$. Now obviously $|\, 2m\rangle$ is an eigenvector of $\exp\{-i\pi L_z/2\}$ with eigenvalue $\exp\{-im\pi/2\}$. In particular, the vectors $|\, 22\rangle$ and $|\, 2-2\rangle$ are degenerate with eigenvalue -1. Hence the Hamiltonian can be restricted to an equivalent 2×2 matrix in the basis $\{|\, 22\rangle, |\, 2-2\rangle\}$. This is the case we are interested in.

To proceed further we must express the Hamiltonian H in the basis $\{|\, 22\rangle, |\, 2-2\rangle\}$. From group theoretical considerations the operator $H(0)$, with octahedral symmetry, has eigenvectors [Butler 1981, p527]

$$\xi_\pm = \sqrt{\tfrac{1}{2}}\,(\mp\,|\, 22\rangle - |\, 2-2\rangle)\,, \tag{8.3}$$

with eigenvalues $E_\pm$. Hence $H(t)$ has eigenvectors

$$\begin{aligned}\xi_\pm(t) &= \mathrm{e}^{-i\omega t L_z}\xi_\pm \\ &= \sqrt{\tfrac{1}{2}}\left(\mp\mathrm{e}^{-2i\omega t}\,|\, 22\rangle - \mathrm{e}^{2i\omega t}\,|\, 2-2\rangle\right),\end{aligned} \tag{8.4}$$

also with eigenvalues $E_\pm$. These relations can be inverted to give

$$|\, 22\rangle = -\sqrt{\tfrac{1}{2}}\mathrm{e}^{2i\omega t}\,(\xi_+(t) - \xi_-(t))\,, \tag{8.5}$$

$$|\, 2-2\rangle = -\sqrt{\tfrac{1}{2}}\mathrm{e}^{-2i\omega t}\,(\xi_+(t) + \xi_-(t))\,. \tag{8.6}$$

Hence, with $E = (E_+ + E_-)/2$ and $\Delta = (E_+ - E_-)/2$, the Hamiltonian has the form

$$H(t) = \begin{bmatrix} E & \Delta\mathrm{e}^{-4i\omega t} \\ \Delta\mathrm{e}^{4i\omega t} & E \end{bmatrix}, \tag{8.7}$$

which is periodic with period $\tilde{t} = \pi/2\omega$. Note that we are using a different basis to that used by Moore and Stedman [1990b]. In summary, by noting that the Hamiltonian $H(t)$ commutes with both L^2 and $\exp\{-i\pi L_z/2\}$ at all times, the problem can be reduced to the finite-dimensional Hilbert space spanned by $\{|\,22\rangle, |\,2-2\rangle\}$. To find the cyclic initial states and Berry phases we use Salzman's formalism with

$$\begin{aligned} A &= \omega L_z \\ &= \begin{bmatrix} 2\omega & 0 \\ 0 & -2\omega \end{bmatrix}, \end{aligned} \tag{8.8}$$

$$\begin{aligned} B &= H(0) - A \\ &= \begin{bmatrix} E - 2\omega & \Delta \\ \Delta & E + 2\omega \end{bmatrix}. \end{aligned} \tag{8.9}$$

The cyclic initial states are just the eigenvectors of B. By direct substitution, one can verify that these are just

$$\phi_\pm(0) = x_\pm \mid 22\rangle + y_\pm \mid 2-2\rangle, \tag{8.10}$$

where $\Delta y_\pm = (2\omega \pm \sqrt{\Delta^2 + 4\omega^2})x_\pm$ and $x_\pm^2 + y_\pm^2 = 1$, and eigenvalues

$$B_\pm = E \mp \sqrt{\Delta^2 + 4\omega^2}. \tag{8.11}$$

Now, as $\exp\{-iA\tilde{t}\} = -1$, the θ_α of equation (5.51) are both equal to $-\pi$. Hence the Berry phases are given by

$$\begin{aligned} \gamma_\pm &= \langle \phi_\pm(0) \mid A \mid \phi_\alpha(0) \rangle - \theta_\pm \\ &= \frac{\pi}{2} \langle \phi_\alpha(0) \mid L_z \mid \phi_\alpha(0) \rangle + \pi \\ &= \pi \left(|x_\pm|^2 - |y_\pm|^2 + 1 \right) \\ &= 2\pi |x_\pm|^2. \end{aligned} \tag{8.12}$$

8.2 The forced harmonic oscillator

To get some feeling for the kind of behaviour possible in infinite-dimensional Hilbert spaces, it is useful to examine the periodically forced harmonic oscillator. This displays extreme behaviour that depends critically on the existence or otherwise of a certain Fourier component in the forcing term. The Hamiltonian is given by [Moore 1990b]

$$H(t) = \omega a^* a + \overline{f}(t)a + f(t)a^* + \beta(t), \tag{8.13}$$

where $f : \mathbb{R} \to \mathbb{C}$ and $\beta : \mathbb{R} \to \mathbb{R}$ are $2\pi/\omega$-periodic and a^* is the creation operator for the oscillator mode.

This problem is solvable using coherent states, which are defined to be the eigenvectors of the annihilation operator: $a \mid z\rangle = z \mid z\rangle$. This is because, as we will now show, the forced harmonic oscillator preserves coherence [Glauber 1966]. The general coherent state $\mid z\rangle$ can be expanded in the usual oscillator number basis $\{\mid n\rangle\}$ as (equation B.8)

$$\mid z\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^2}{\sqrt{n!}} \mid n\rangle. \tag{8.14}$$

Now imagine that z is a time-dependent parameter. In the following we will need the explicit form of $(\mathrm{d}/\mathrm{d}t) \mid z\rangle$. We have that

$$\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{d}t} \mid z\rangle &= \tfrac{\mathrm{d}}{\mathrm{d}t} \sum_{n=0}^{\infty} \mathrm{e}^{-z\overline{z}/2} \frac{z^2}{\sqrt{n!}} \mid n\rangle \\
&= \sum_{n=0}^{\infty} -\tfrac{1}{2}\left(\dot{z}\overline{z} + z\dot{\overline{z}}\right) \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \mid n\rangle + \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{n\dot{z}z^{n-1}}{\sqrt{n!}} \mid n\rangle \\
&= -\tfrac{1}{2}\left(\dot{z}\overline{z} + z\dot{\overline{z}}\right) \mid z\rangle + \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \sqrt{n+1} \frac{\dot{z}z^n}{\sqrt{n!}} \mid n+1\rangle.
\end{aligned} \tag{8.15}$$

Now

$$a^* \mid z\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \sqrt{n+1} \frac{z^n}{\sqrt{n!}} \mid n+1\rangle, \tag{8.16}$$

so that, comparing equations (8.14) and (8.15)

$$\tfrac{\mathrm{d}}{\mathrm{d}t} \mid z\rangle = -\tfrac{1}{2}\left(\dot{z}\overline{z} + z\dot{\overline{z}}\right) \mid z\rangle + \dot{z}a^* \mid z\rangle. \tag{8.17}$$

We are now in a position to prove that H preserves coherence. Consider the initial state $\phi(0) =\mid z(0)\rangle$. For the evolved state we try

$$\phi(t) = \mathrm{e}^{\mathrm{i}\theta(t)} \mid z(t)\rangle, \tag{8.18}$$

where

$$z(t) = \mathrm{e}^{-\mathrm{i}\omega t}\big(z(0) - \mathrm{i}\int_0^t f(t')\mathrm{e}^{\mathrm{i}\omega t'}\,\mathrm{d}t'\big), \tag{8.19}$$

$$\theta(t) = -\int_0^{\tilde{t}} \left(\beta + \tfrac{1}{2}\left(\overline{f}z + f\overline{z}\right)\right)\,\mathrm{d}t. \tag{8.20}$$

Note that θ is real as required. In fact, all we need are the differential equations satisfied by z and θ:

$$\dot{z} = -\mathrm{i}(\omega z + f), \tag{8.21}$$

$$\dot{\theta} = -\beta - \tfrac{1}{2}\left(\overline{f}z + f\overline{z}\right). \tag{8.22}$$

Note that equation (8.21) is just the classical equation of motion. Using equation (8.18), the time-dependent Schrödinger equation is equivalent to

$$\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t} \mid z\rangle = \dot{\theta} \mid z\rangle + H \mid z\rangle. \tag{8.23}$$

Substituting equations (8.17) and (8.22) we then have

$$\begin{aligned}
\mathrm{LHS} &= -\tfrac{\mathrm{i}}{2}\left(-\mathrm{i}(\omega z + f)\overline{z} + \mathrm{i}(\omega\overline{z} + \overline{f})z\right) \mid z\rangle + (\omega z + f)a^* \mid z\rangle \\
&= \tfrac{1}{2}\left(\overline{f}z - f\overline{z}\right) \mid z\rangle + (\omega z + f)a^* \mid z\rangle, \qquad (8.24) \\
\mathrm{RHS} &= \left(-\beta - \tfrac{1}{2}\left(\overline{f}z + f\overline{z}\right)\right) \mid z\rangle + (\omega z + f)a^* \mid z\rangle + \left(\overline{f}z + \beta\right) \mid z\rangle \\
&= \tfrac{1}{2}\left(\overline{f}z - f\overline{z}\right) \mid z\rangle + (\omega z + f)a^* \mid z\rangle \\
&= \mathrm{LHS}. \qquad (8.25)
\end{aligned}$$

Hence we can see that an arbitrary coherent initial state remains coherent throughout its evolution.

We now investigate whether or not any of the initial states $\mid z(0)\rangle$ are cyclic. This will then be generalised to all initial states. From equation (8.18) and with $\tilde{t} = 2\pi/\omega$, we have that

$$\phi(\tilde{t}) = \mathrm{e}^{\mathrm{i}\theta(\tilde{t})} \mid z(\tilde{t})\rangle. \tag{8.26}$$

Now, from equation (B.20), the inner product of any two coherent states has square modulus

$$|\langle z' \mid z\rangle|^2 = \mathrm{e}^{-|z'-z|^2}. \tag{8.27}$$

As this is always less than unity for $z \neq z'$, no two distinct coherent states can be equal up to a phase. Note that as (8.27) is always greater than zero, no two coherent states can be orthogonal either. Thus the initial state $\mid z(0)\rangle$ is cyclic iff $z(0) = z(\tilde{t})$. Substituting into equation (8.19), and using the fact that $\exp\{-\mathrm{i}\omega\tilde{t}\} = 1$, we require that

$$\begin{aligned} z(0) &= z(\tilde{t}) \\ &= z(0) - \mathrm{i}\int_0^{\tilde{t}} f(t)\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t \\ \Rightarrow \qquad 0 &= \int_0^{\tilde{t}} f(t)\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t. \end{aligned} \tag{8.28}$$

Now f is $\tilde{t}$-periodic and so we can expand it in a Fourier series:

$$f(t) = \sum_{n=0}^{\infty} f^{[n]}\mathrm{e}^{\mathrm{i}\omega t}, \tag{8.29}$$

whereupon the condition (8.28) is equivalent to the vanishing of the Fourier component $f^{[-1]}$. In other words, the behaviour of the system depends crucially on the existence or otherwise of the Fourier component $f^{[-1]}$. If it vanishes then all initial coherent states are cyclic, whereas if it is non-zero there do not exist any cyclic coherent states. In the next few paragraphs I will strengthen these conclusions. We will see that the conclusions just reached hold for arbitrary states.

First consider the case $f^{[-1]} = 0$. Then all coherent states are cyclic. Now we will see that they all have the same overall phase. But this means that any linear combination of them is also a cyclic initial state with the same overall phase. Then, as the coherent states are a complete (in fact overcomplete) set, all initial states are cyclic with the same overall phase. This is the ultimate example of quasi-degeneracy. That the coherent states all have the same overall phase follows from the decomposition formalism of section 5.1. If we write the evolution operator as $U = Z\exp\{\mathrm{i}Mt\}$, then the cyclic initial states are the eigenvectors of M and the overall phases are the corresponding eigenvalues of $M\tilde{t}$. Now if two coherent states had different overall phases, they would belong to distinct eigenspaces of M and so would be orthogonal. However, in light of equation (8.27) this is impossible. Thus the coherent states must all have the same overall phase.

It is instructive to show this directly from equation (8.20), which defines the phase θ. Substituting $t = \tilde{t}$ we have

$$\theta(\tilde{t}) = -\int_0^{\tilde{t}} \left(\tfrac{1}{2}\left(f\overline{z} + \overline{f}z\right) + \beta\right) \mathrm{d}t. \tag{8.30}$$

To show that this is independent of $z(0)$ it suffices to show that $\int_0^{\tilde{t}} f\overline{z}\,\mathrm{d}t$ is independent of $z(0)$. Now, substituting equation (8.19), we have

$$f\overline{z} = f\mathrm{e}^{\mathrm{i}\omega t}\left(\overline{z}(0) + \mathrm{i}\int_0^t \overline{f}\mathrm{e}^{-\mathrm{i}\omega t'}\,\mathrm{d}t'\right)$$

$$\Rightarrow \quad \int_0^{\tilde{t}} f\overline{z}\,\mathrm{d}t = \overline{z}(0)\int_0^{\tilde{t}} f\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t + \mathrm{i}\int_0^{\tilde{t}}\left(f\mathrm{e}^{\mathrm{i}\omega t}\int_0^t \overline{f}\mathrm{e}^{-\mathrm{i}\omega t'}\,\mathrm{d}t'\right)\mathrm{d}t. \tag{8.31}$$

However, by assumption $(1/\tilde{t})\int_0^{\tilde{t}} f\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t = f[-1]$ is zero, so that equation (8.31) simplifies to

$$\int_0^{\tilde{t}} f\overline{z}\,\mathrm{d}t = \mathrm{i}\int_0^{\tilde{t}}\left(f\mathrm{e}^{\mathrm{i}\omega t}\int_0^t \overline{f}\mathrm{e}^{-\mathrm{i}\omega t'}\,\mathrm{d}t'\right)\mathrm{d}t, \tag{8.32}$$

which is manifestly independent of $z(0)$ as required. To find the Berry phases we need merely note that $|\, z(t)\rangle$ is a single-valued vector. Substituting into equation

(3.8) and using (8.17) gives

$$\begin{aligned}\gamma &= \mathrm{i}\int_0^{\tilde{t}} \langle z(t) \mid \tfrac{\mathrm{d}}{\mathrm{d}t} \mid z(t)\rangle \,\mathrm{d}t \\ &= \mathrm{i}\int_0^{\tilde{t}} \langle z \mid -\tfrac{1}{2}\left(\dot{z}\overline{z} + \dot{\overline{z}}z\right) + \dot{z}a^* \mid z\rangle \,\mathrm{d}t \\ &= \tfrac{\mathrm{i}}{2}\int_0^{\tilde{t}} \left(\dot{z}\overline{z} - \dot{\overline{z}}z\right)\,\mathrm{d}t. \end{aligned} \tag{8.33}$$

Note that by substituting $\dot{z} = -\mathrm{i}(\omega z + f)$, we recover the result of Moore [1990b]. This can readily be evaluated in terms of the known Fourier components of f. Let $f = \sum_n f^{[n]}\exp\{in\omega t\}$. Now z is $\tilde{t}$-periodic so that it too has a Fourier decomposition: $z = \sum_n z^{[n]}\exp\{in\omega t\}$. Substituting into equation (8.21) we have

$$\begin{aligned} -\sum_n n\omega z^{[n]}\mathrm{e}^{in\omega t} &= \sum_n \omega z^{[n]}\mathrm{e}^{in\omega t} + \sum_n f^{[n]}\mathrm{e}^{in\omega t} \\ \Rightarrow \qquad (n+1)\omega z^{[n]} &= f^{[n]}. \end{aligned} \tag{8.34}$$

Now the coefficient of $z^{[-1]}$ vanishes, as does $f^{[-1]}$. Hence $z^{[-1]}$ is arbitrary. Note that this is where the assumption that $f^{[-1]} = 0$ is necessary. This is because if $f^{[-1]}$ does not vanish, then the equation for $z^{[-1]}$ is inconsistent, meaning that no periodic solution for z can exist. For $n \neq -1$, equation (8.34) gives

$$z^{[n]} = \frac{f^{[n]}}{(n+1)\omega}. \tag{8.35}$$

To find $z^{[-1]}$ in terms of the known $z(0)$ we subsitute $t = 0$ into the Fourier decomposition of z. This gives

$$\begin{aligned} z(0) &= \sum_{n\neq -1} \frac{f^{[n]}}{(n+1)\omega} + z^{[-1]} \\ \Rightarrow \qquad z^{[-1]} &= z(0) - \sum_{n\neq -1} \frac{f^{[n]}}{(n+1)\omega}. \end{aligned} \tag{8.36}$$

To evaluate equation (8.33), we need $\int_0^{\tilde{t}} \dot{z}\overline{z}\,\mathrm{d}t$. Now

$$\begin{aligned} \dot{z}\overline{z} &= \sum_{n,m} \mathrm{i}n\omega z^{[n]}\overline{z}^{[m]}\mathrm{e}^{\mathrm{i}(n-m)\omega t} \\ \Rightarrow \qquad \int_0^{\tilde{t}} \dot{z}\overline{z}\,\mathrm{d}t &= \sum_n 2\pi \mathrm{i}n|z^{[n]}|^2. \end{aligned} \tag{8.37}$$

Hence

$$\gamma = -2\pi \sum_n n|z^{[n]}|^2. \tag{8.38}$$

We now turn to the case when $f^{[-1]}$ does not vanish. I will show that, not only do no coherent cyclic initial states exist, but there are in fact no cyclic initial states at all. Put $k = \tilde{t}f^{[-1]}$ so that, from equation (8.19), $z(\tilde{t}) = z(0) - \mathrm{i}k$. In the case where $f^{[-1]} = 0$ which was discussed above, the phase $\theta(\tilde{t})$ did not depend on the initial states $\mid z(0)\rangle$. In our case however, this is no longer true. Further, it is the fact that $\theta(\tilde{t})$ now depends on $\mid z(0)\rangle$ that forbids the initial states from being cyclic. To prove this assertion we need $\int_0^{\tilde{t}} f\overline{z}\,\mathrm{d}t$. Following the proof of equation (8.32) we find that

$$\int_0^{\tilde{t}} f\overline{z}\,\mathrm{d}t = \overline{z}(0)k + \mathrm{i}\int_0^{\tilde{t}} \left(f\mathrm{e}^{\mathrm{i}\omega t} \int_0^t \overline{f}\mathrm{e}^{-\mathrm{i}\omega t'}\,\mathrm{d}t' \right) \mathrm{d}t. \tag{8.39}$$

Hence, from equation (8.30),

$$\begin{aligned} \theta(\tilde{t}) &= -\int_0^{\tilde{t}} \left(\tfrac{1}{2}\left(f\overline{z} + \overline{f}z\right) + \beta\right) \mathrm{d}t \\ &= -\tfrac{1}{2}\left(\overline{z}(0)k + z(0)\overline{k} + \alpha\right), \end{aligned} \tag{8.40}$$

where α is independent of $z(0)$. In section B.1, I show that the coherent states give the spectral resolution of unity

$$1 = \tfrac{1}{\pi}\int \mathrm{d}^2 z \mid z\rangle\langle z \mid \tag{8.41}$$

so that an arbitrary initial state $\phi(0)$ can be written

$$\phi(0) = \tfrac{1}{\pi}\int \mathrm{d}^2 z b(z) \mid z\rangle, \tag{8.42}$$

where $b(z) = \langle z \mid \phi(0)\rangle$. Now imagine that $\phi(0)$ is a cyclic initial state with overall phase χ: $\phi(\tilde{t}) = \exp\{\mathrm{i}\chi\}\phi(0)$. I will show that this leads to an inconsistency. From equations (8.30) and (8.40), $\psi_z(0) =\mid z\rangle$ evolves into

$$\psi_z(\tilde{t}) = \mathrm{e}^{-\mathrm{i}(\overline{z}k + z\overline{k})/2}\mathrm{e}^{\mathrm{i}\alpha} \mid z - \mathrm{i}k\rangle, \tag{8.43}$$

where α is independent of z. Thus $\phi(0)$ evolves into

$$\phi(\tilde{t}) = \tfrac{1}{\pi}\int \mathrm{d}^2 z b(z) \mathrm{e}^{\mathrm{i}\alpha} \mathrm{e}^{-\mathrm{i}(\overline{z}k + z\overline{k})/2} \mid z - \mathrm{i}k\rangle. \tag{8.44}$$

Now let $\phi'(0) = (1/\pi)\int \mathrm{d}^2 z b(z) \mid z + a\rangle$ for some arbitrary complex number a. Then, as α does not depend on z,

$$\begin{aligned}\phi'(\tilde{t}) &= \tfrac{1}{\pi}\int \mathrm{d}^2 z b(z) \mathrm{e}^{\mathrm{i}\alpha} \mathrm{e}^{-\mathrm{i}\left((\overline{z}+\overline{a})k + (z+a)\overline{k}\right)/2} \mid z - \mathrm{i}k + a\rangle \\ &= \mathrm{e}^{-\mathrm{i}(\overline{a}k + a\overline{k})} \tfrac{1}{\pi}\int \mathrm{d}^2 z b(z) \mathrm{e}^{\mathrm{i}\alpha} \mathrm{e}^{-\mathrm{i}(\overline{z}k + z\overline{k})/2} \mid z - \mathrm{i}k + a\rangle. \end{aligned} \tag{8.45}$$

But, using equation (8.44) and the fact that $\phi(\tilde{t}) = \exp\{\mathrm{i}\chi\}\phi(0)$, we can see that

$$\phi'(\tilde{t}) = \mathrm{e}^{-\mathrm{i}(\overline{a}k + a\overline{k})/2} \mathrm{e}^{\mathrm{i}\chi} \phi'(0). \tag{8.46}$$

Hence $\phi'(0)$ is also a cyclic initial state, but with the overall phase $\chi' = \chi - (\overline{a}k + a\overline{k})/2$. Further, if we let a run over C, then χ' will run over the entire half-open interval $[0, 2\pi)$. But each distinct overall phase corresponds to an eigenspace of the operator M, with different eigenspaces being orthogonal. This means that, as $[0, 2\pi)$ is uncountable, there is an uncountable set of linearly independent vectors in the Hilbert space $\mathcal{H}$ of the oscillator. But this is impossible as $\mathcal{H}$ is assumed to be separable [Young 1988, p38]. Thus our initial assumption that $\phi(0)$ was a cyclic initial state must have been false.

To recapitulate, the periodically forced harmonic oscillator displays extreme behaviour that depends critically on the existence or otherwise of a certain Fourier component in the forcing term. If it is present then no states are cyclic, whereas if it is not they all are. Thus, for example, the sinusoidally forced oscillator has no cyclic initial states. These results will be verified in the next section, when I discuss functional analytic approaches to the existence problem. Coherent states have also been used in the investigation of Berry phase in several other ways. For example, Chaturvedi *et al.* [1987] use them to solve the problem of the displaced harmonic oscillator with adiabatically varying parameter. This was discussed in more detail in section 4.2. Also, Brihaye *et al.* [1990] analyse Hamiltonians which are expressible in terms of the generators of a given Lie algebra by using coherent states. This example was discussed in section 7.2.

8.3 Functional analytic results

In this section I discuss the application of functional analysis to the problem of the existence of cyclic initial states. This makes use of the concept of a bound state. These are essentially states that stay in a bounded region of space uniformly in time. This will be made more precise soon. We find that, under certain conditions, the space spanned by the cyclic initial states is precisely the set of bound states. Hence if all states are bound, there must be a complete set of cyclic initial states. This theorem can be easily applied to many systems. For example, it allows us to verify the results derived in the last section for the forced harmonic oscillator.

We must first define the bound states. Let the system of interest have Hilbert space $L^2(\mathbb{R}^n, \mathrm{d}^n x)$ and let $\mathcal{M}$ be a subset of $\mathbb{R}^n$. We define the operator $F(\mathcal{M})$ as the operator of multiplication by the characteristic function of $\mathcal{M}$. Then, if the system has Hamiltonian H and evolution operator U, the state ϕ is called *bound* iff

$$\lim_{R\to\infty} \sup_{t>0} \|F(|x| > R)U(t)\phi\| = 0. \tag{8.47}$$

In contrast, ϕ is called *propagating* iff for all R,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \|F(|x| < R)U(t)\phi\| \, \mathrm{d}t = 0. \tag{8.48}$$

To motivate our discussion, let the Hamiltonian be time-independent so that $U = \exp\{-\mathrm{i}Ht\}$. We decompose the Hilbert space into the direct sum

$$\mathcal{H} = \mathcal{H}^p \oplus \mathcal{H}^c, \tag{8.49}$$

where the point spectral subspace $\mathcal{H}^p$ is spanned by the eigenvectors of H and $\mathcal{H}^c$ is the continuous spectral subspace. Then one can prove that the bound states are precisely the elements of $\mathcal{H}^p$ and the propagating states are precisely the elements of $\mathcal{H}^c$. This is the RAGE theorem [Reulle 1969]. Now, as the Hamiltonian is time-independent, the spectral properties of the evolution operator $U(t)$ are preciseley the same as those of the Hamiltonian. In particular, the eigenvectors

of the monodromy operator $U(\tilde{t})$ span the space $\mathcal{H}^p$. But these eigenvectors are precisely the cyclic initial states. Hence, for the time-independent case, there are as many cyclic initial states as eigenvectors of the Hamiltonian. This is obvious, as these are just the stationary states.

The utility of all of this theory only becomes clear when the Hamiltonian is made time-dependent. In this case, the spectral properties of $H(t)$ and $U(t)$ are not simply related. Further the RAGE theorem is not satisfied. However, a modified form still holds. This states that for $\tilde{t}$-periodic Hamiltonians satisfying a certain condition to be specified later, the bound states are precisely the states in the space spanned by the eigenvectors of the monodromy operator $U(\tilde{t})$. Note the differences to the time-independent version. In the time-independent case, an arbitrary Hamiltonian could be used. For the periodic case however, the class of Hamiltonians for which the theorem holds is restricted. Secondly, and more importantly, in the time-independent case the spaces spanned by the eigenvectors of the evolution operator and the Hamiltonian were identical. Thus the theorem could be stated in terms of either. Here the spaces can differ. The fact that the space spanned by the eigenvectors of the monodromy operator turns out to be the one used in the theorem is of critical importance. This is because this space is precisely the one spanned by the cyclic initial states. Thus, the existence of a bound state guarantees the existence of a cyclic initial state. For example, if all of the states are bound then, as with the time-independent case, there is a complete set of cyclic initial states. This result also holds for real systems of differential equations [Yoshizawa 1975, p164].

The subsidiary condition we need is most easily stated using Moore and Stedman's evolution operator decomposition $U = Z\exp\{\mathrm{i}Mt\}$. Then the theorem is satisfied if $F(|x| < R)(\mathrm{i} - M)^{-1}$ is compact for all R [Enss and Veselić 1983]. This condition can be converted into one on the Hamiltonian itself [Yajima and Kitada 1983]. Yajima and Kitada show that it is sufficient that H be of the form $H(t) = -\nabla^2/2 + V_1(t) + V_2(t)$, where V_1 and V_2 are both symmetric and $\tilde{t}$-periodic and satisfy the following conditions. V_1 is continuously differentiable and bound-

ed. $V_2(t)$ is the operator of multiplication by an $L^p(\mathbb{R}^n) \cap L^q(\mathbb{R}^2)$ function with $1 \leq p < n/2 < q \leq \infty$. Gesztesy and Mitter [1981] note that the eigenvectors of $U(\tilde{t})$ are only cyclic initial states if they are also in the domain of $H(0)$. However, the usual conditions imposed upon $H(t)$ in order to guarantee the existence of the evolution operator (see section 2.2) include forcing H to have a time-independent domain, which is then also the domain of $U(t)$. Thus the eigenvectors of the monodromy operator must be in the domain of $H(0)$ as required.

This formalism can be applied to several important problems. For instance, Combescure [1990] discusses periodically kicked Hamiltonians. Another example is afforded by the sinusoidally forced harmonic oscillator $H = -p^2/2 + \omega^2 x^2/2 + x \sin \omega_0 t$. Enss and Veselić [1983] show that there are two possibilities. If $\omega_0 = \omega$ then there are no bound states and so there are no cyclic initial states. This verifies the analysis of the last section. However, if $\omega_0 \neq \omega$, then all states are bound and so there is a complete set of cyclic initial states. Hence, as was the case with the general forced harmonic oscillator discussed above, there is either a complete set of cyclic initial states or none at all. Hagedorn *et al.* [1986] have shown that this result holds for all Hamiltonians of the form

$$H(t) = \alpha(t)p^2 + \beta(t)(p \cdot q + q \cdot p) + \gamma(t)q^2 + \delta(t)p + \epsilon(t)q + \zeta(t), \quad (8.50)$$

where the coefficients are real and piecewise continuous.

Another interesting example is given by Huang [1989]. He considered Hamiltonians of the form

$$H(t) = -\tfrac{\mathrm{d}^2}{\mathrm{d}x^2} + f(t)x^2 \quad (8.51)$$

on $L^2(\mathbb{R}, \mathrm{d}x)$, where $f \not\equiv 0$ is real, $\tilde{t}$-periodic and piecewise continuous. Let f_+ be the positive part of f:

$$f_+(t) = \begin{cases} f(t) & : f(t) \geq 0 \\ 0 & : f(t) < 0 \end{cases}. \quad (8.52)$$

Then the Hamiltonian (8.51) has a complete set of cyclic initial states if $\int_0^{\tilde{t}} f(t)\,\mathrm{d}t \geq$

0 and $\int_0^{\tilde{t}} f_+(t)\,\mathrm{d}t \leq \frac{1}{\tilde{t}}$. An example of a Hamiltonian not satisfying these conditions and not having any cyclic initial states is the one with

$$f(t) = \begin{cases} \omega^2 & : 0 \leq t < c \\ 0 & : c \leq t < \tilde{t} \end{cases}, \tag{8.53}$$

where $c = \pi/2\omega < \tilde{t}$. This has

$$\int_0^{\tilde{t}} f_+(t)\,\mathrm{d}t = \frac{\pi\omega}{2} > \frac{\pi^2}{4\tilde{t}} > \frac{1}{\tilde{t}}. \tag{8.54}$$

The final application I will discuss is the stability of the bound states. If we have a Hamiltonian whose monodromy operator $U(\tilde{t})$ is pure point, that is a system with a complete set of cyclic initial states, it is of interest to find the class of $\tilde{t}$-periodic perturbations which preserve this property. It is convenient to take the unperturbed Hamiltonian as being time-independent and pure point. Then, by the RAGE theorem, there is a complete set of cyclic initial states.

Enss and Veselić [1983] discuss two interesting applications. For the first, let the unperturbed Hamiltonian be the harmonic oscillator. Then any $2\pi/\omega$-periodic uniformly bounded perturbation $V(t)$ that is continuous in t preserves the completeness of the set of cyclic initial states. Note that this seems to contradict the forced harmonic oscillator example considered above. There it was precisely when the period of the perturbation matched the natural period $2\pi/\omega$ of the oscillator that the bound states disappeared. However, in that case the perturbation $x \sin\omega_0 t$ was not bounded and so much more singular. Enss and Veselić also use this method to prove the existence of cyclic inital states for the spherically symmetric atom in a circularly polarised radiation field, verifying the results of section 5.3 achieved using Salzman's evolution operator decomposition.

This perturbation theoretic approach was also used by Howland [1989] in a probabilistic sense. Let the time-independent unperturbed Hamiltonian H_0 have eigenvectors ξ_n and eigenvalues λ_n, where $\lambda_{n+1} - \lambda_n > \alpha n^{2+\epsilon}$ for some positive α and ϵ. We need the following definition. An operator A is *strongly H-finite* iff $\sum_n |A\xi_n| < \infty$. Now let the perturbation $V(t)$ be of the form $V(t) = A^* W(t) A^*$,

where A is strongly H-finite and W is uniformly bounded, $\tilde{t}$-periodic and positive. Then the Hamiltonian $H(t) = H_0 + \beta V(t)$ has a complete set of cyclic initial states for almost all β.

These results show the power of the functional analytic approach. This method characterises the existence of cyclic initial states in terms of the existence of geometrically bound states, and can be used (among other things) to discuss the perturbative stability of cyclic initial states. However, it would be useful to find a more readily testable requirement for the existence of cyclic initial states, perhaps in terms of the spectral decomposition of the Hamiltonian.

Chapter Nine

Applications to quantum optics

In the preceding eight chapters I have frequently used the semi-classical Jaynes-Cummings model (a two-level atom in a radiation field in the rotating wave approximation) as an example. In fact the Berry phase has many applications in the field of quantum optics. These applications are the subject of this chapter. For example, in section 9.1 I show that the Berry phases of the Jaynes-Cummings model can be interpreted in terms of the frequency of the Rabi oscillation and the splitting of the Mollow triplet, both well known quantities in quantum optics [Cohen-Tannoudji 1977]. This involves the Fourier theory of chapter 6, exploiting the relationship between the Floquet Hamiltonian K and the joint electron-photon Hamiltonian H_j and was first reported by Moore [1990b].

Having shown how the Rabi oscillations of the semi-classical two-level atom can be interpreted in terms of the overall phases of the system, in section 9.2 I discuss the oscillations themselves. This work was first reported by Moore [1990c]. Given an arbitrary initial state $\phi(0)$, the probability P_+ of finding the system in the upper atomic state is a π/k-periodic function of time. Now, as I will discuss in section 11.5, the definition of Berry phases holds even when the Hamiltonian is not itself periodic. Thus we are not barred from calculating the Berry phases that arise for evolution from time $t = 0$ to time $t = \pi/k$. However we find that, even though the probability P_+ is π/k-periodic, the state itself is only periodic (up to a phase) if we start in either the upper or lower atomic state. Therefore, to extract the phase relationship between general initial and final states we must use the Pancharatnam phase [Samuel and Bhandari 1988]. This is discussed in more detail in section 11.2, where an alternative definition that makes the overall

phase an observable (self-adjoint operator) is discussed.

I then move to the fully quantum mechanical model. Using the concept of quasi-degeneracy developed in section 5.2, we find that any initial state formed as a linear combination of the vectors $\{|+,n\rangle, |-,n+1\rangle\}$ for some fixed n is cyclic with period $\pi(\lambda\sqrt{n+1})^{-1}$. While this is in sharp contrast to the semi-classical case, it is not a fair comparison. This is because the quantum mechanical state most closely corresponding to the semi-classical initial state $\phi(0)$ is the product of that state with a photon coherent state (see section B.2) and not a linear combination of $|+,n\rangle$ and $|-,n+1\rangle$. However, when we analyse the system with initial states of this form, we find that it still behaves differently to the semi-classical limit. The Rabi oscillations are no longer exact, being subject to collapses and revivals.

If these collapses and revivals were themselves perfect, we could find their Berry phases in the same way as we did for the semi-classical Rabi oscillations. However they are not. This is because the eigenvalues of the quantum Hamiltonian involve terms in $\sqrt{n+1}$. With this in mind, we then study the quantum optical model consisting of two degenerate electronic levels coupled through a virtual level by a Raman transition [Phoenix and Knight 1990]. For this system the eigenvalues involve terms in $n+1$ and so the collapses and revivals are perfect. However, we find that the wavefunctions are not cyclic over the period of one collapse and revival, just as in the semi-classical Jaynes-Cummings model they were not cyclic over the period of one complete Rabi oscillation. Thus we must again invoke the Pancharatnam phase.

The analysis of sections 9.1 and 9.2 uses the simplest model available. For example, I ignore the non-rotating wave contributions and the effects of spontaneous emission. In section 9.3 I discuss the impact of these approximations, showing the way for some future work.

9.1 Interpretation of the Rabi oscillation

In previous chapters I have used the Jaynes-Cummings model as an example. However we can go a lot further. In this section I will show how the Berry phases can be interpreted in terms of two well known observables, the frequency of the Rabi oscillation and the splitting of the Mollow triplet. This work was first reported by Moore [1990b]. Similar results have been obtained by Tewari [1989] in the adiabatic context.

This interpretation is based upon the formal similarity between the joint electron-photon Hamiltonian

$$H_j = \tfrac{\omega}{2}\sigma_z + \omega b^* b + \lambda(b^*\sigma_- + b\sigma_+), \tag{9.1}$$

and the Floquet Hamiltonian discussed in section 6.2

$$K = -\mathrm{i}\tfrac{\partial}{\partial t} + H(t), \tag{9.2}$$

where $H(t)$ is the semi-classical Hamiltonian

$$H(t) = \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix} \tag{9.3}$$

derived as an asymptotic limit in section 2.2. This formal similarity has been discussed by Shirley [1965] and Casati [1989].

To display the relationship between H_j and K explicitly, we write both Hamiltonians as matrices:

$$H_j = \begin{array}{c} \\ 2- \\ 1+ \\ 1- \\ 0+ \\ 0- \end{array} \begin{array}{c} \begin{array}{ccccccc} & & 2- & 1+ & 1- & 0+ & 0- \end{array} \\ \begin{bmatrix} \ddots & \ddots & \ddots & & & & 0 \\ & 0 & \frac{3\omega}{2} & \sqrt{2}\lambda & & & \\ & & \sqrt{2}\lambda & \frac{3\omega}{2} & 0 & & \\ & & & 0 & \frac{\omega}{2} & \sqrt{1}\lambda & \\ & & & & \sqrt{1}\lambda & \frac{\omega}{2} & 0 \\ & & & & & 0 & -\frac{\omega}{2} \end{bmatrix} \end{array}, \tag{9.4}$$

$$K = \begin{array}{c} \\ 1+ \\ 1- \\ 0+ \\ 0- \\ \\ \end{array} \begin{array}{c} \begin{array}{cccccccc} & & 1+ & 1- & 0+ & 0- & & \end{array} \\ \begin{bmatrix} \ddots & \ddots & \ddots & & & & & 0 \\ & k & \frac{3\omega}{2} & 0 & & & & \\ & & 0 & \frac{\omega}{2} & k & & & \\ & & & k & \frac{\omega}{2} & 0 & & \\ & & & & 0 & -\frac{\omega}{2} & k & \\ 0 & & & & & \ddots & \ddots & \ddots \end{bmatrix} \end{array}. \tag{9.5}$$

There are only two differences. First, the label n for H_j must be non-negative, whereas it can be any integer for K. Second, the off-diagonal elements of H_j involve terms of the form $\sqrt{n}\lambda$ whereas the corresponding elements of K involve k. However these differences are physically illusory. To get the semi-classical limit the initial state must be the direct product of an atomic state and a photon coherent state $\mid z\rangle$. Further, $|z|$ must be large. As $|z|$ grows, the Poisson distribution of photon number state occupancies becomes strongly peaked about $n = |z|^2$. This means that only those components of the evolving state with n close to $|z|^2$ contribute to any measurable quantities. In other words, we can ignore the basis vectors $\mid n\rangle$ that are not close to $n = |z|^2$. Further, we can replace $\sqrt{n}$ by its mean value $|z|$. But this means that we can replace $\sqrt{n}\lambda$ by the effective coupling constant k. Thus the two Hamiltonian are physically equivalent.

We can now physically interpret the Berry phase. We note that, as K and H_j are physically equivalent, the quasi-energies (eigenvalues of K) are equal to the eigenvalues of H_j. We start with the Rabi oscillation. Consider the arbitrary initial state

$$\phi(0) = \mid z\rangle(a_+ \mid +\rangle + a_- \mid -\rangle) \tag{9.6}$$

of the joint Hamiltonian H_j. To find its evolution we express it in the eigenbasis $\{\mid \epsilon_{\pm,n}\rangle\}$ of H_j. By direct substitution, one can readily verify that this basis is given by

$$\mid \epsilon_{\pm,n}\rangle = \pm\sqrt{\tfrac{1}{2}} \mid +, n\rangle + \sqrt{\tfrac{1}{2}} \mid -, n+1\rangle, \tag{9.7}$$

$$\epsilon_{\pm,n} = (n + \tfrac{1}{2})\omega \pm \lambda\sqrt{n+1}. \tag{9.8}$$

In the following I will frequently ignore the $n = 0$ terms in the expansion of the coherent state in equation (9.6). This is justifiable as, since $|z|$ is large, they are negligibly small. With this in mind, and using the fact that $z \sim \exp\{i\alpha\}\sqrt{n}$ for some phase α, we have

$$\begin{aligned}\phi(0) &= \sum_{n=0}^{\infty} e^{-|z|^2/2}\frac{z^n}{\sqrt{n!}}(a_+ \mid +,n\rangle + a_- \mid -,n\rangle) \\ &= \sum_{n=0}^{\infty}\sqrt{\tfrac{1}{2}}e^{-|z|^2/2}\frac{z^n}{\sqrt{n!}}((a_+ + e^{i\alpha}a_-) \mid \epsilon_{+,n}\rangle \\ &\qquad + (-a_+ + e^{i\alpha}a_-) \mid \epsilon_{-,n}\rangle).\end{aligned} \tag{9.9}$$

Hence the evolved state is given by

$$\begin{aligned}\phi(t) &= \sum_{n=0}^{\infty}\sqrt{\tfrac{1}{2}}e^{-|z|^2/2}\frac{z^n}{\sqrt{n!}}((a_+ + e^{i\alpha}a_-)e^{-i\epsilon_{+,n}t} \mid \epsilon_{+,n}\rangle \\ &\qquad + (-a_+ + e^{i\alpha}a_-)e^{-i\epsilon_{-,n}t} \mid \epsilon_{-,n}\rangle) \\ &= \sum_{n=0}^{\infty}\tfrac{1}{2}e^{-|z|^2/2}\frac{z^n}{\sqrt{n!}}(a_{+,n}(t) \mid +,n\rangle + a_{-,n}(t) \mid -,n\rangle).\end{aligned} \tag{9.10}$$

Thus the probability of finding the system in the state $\mid +,n\rangle$ is given by

$$\begin{aligned}P_{+,n} &= \tfrac{1}{4}e^{-|z|^2}\frac{|z|^{2n}}{n!}|a_{+,n}|^2 \\ &= \tfrac{1}{4}e^{-|z|^2}\frac{|z|^{2n}}{n!}|a_+(e^{-i\epsilon_{+,n}t} + e^{-i\epsilon_{-,n}t}) + e^{i\alpha}a_-(e^{-i\epsilon_{+,n}t} - e^{-i\epsilon_{-,n}t})|^2 \\ &= \tfrac{1}{2}e^{-|z|^2}\frac{|z|^{2n}}{n!}\big(1 + (|a_+|^2 - |a_-|^2)\cos(\epsilon_{+,n} - \epsilon_{-,n})t \\ &\qquad + i(e^{-i\alpha}\overline{a}_-a_+ - e^{i\alpha}\overline{a}_+a_-)\sin(\epsilon_{+,n} - \epsilon_{-,n})t\big).\end{aligned} \tag{9.11}$$

Now, as we can replace $\sqrt{n}$ by $|z|$, the $\epsilon_{+,n} - \epsilon_{-,n}$ are independent of n. Thus we can easily evaluate the probability of finding the system in the upper atomic state. We have

$$\begin{aligned}P_+ &= \sum_{n=0}^{\infty} P_{+,n} \\ &= \tfrac{1}{2}\big(1 + (|a_+|^2 - |a_-|^2)\cos(\epsilon_{+,n} - \epsilon_{-,n})t \\ &\qquad + i(e^{-i\alpha}\overline{a}_-a_+ - e^{i\alpha}\overline{a}_+a_-)\sin(\epsilon_{+,n} - \epsilon_{-,n})t\big).\end{aligned} \tag{9.12}$$

This is manifestly periodic with frequency $\epsilon_{+,n} - \epsilon_{-,n}$. This is the Rabi oscillation [Knight and Milonni 1980]. Hence the frequency of the Rabi oscillation is just the difference between the eigenvalues $\epsilon_{+,n}$ and $\epsilon_{-,n}$. But, due to the relationship between H_j and K, these eigenvalues are just the quasi-energies of the Floquet Hamiltonian. Further these are precisely the overall phases of the two atomic cyclic initial states (up to a factor of $-\tilde{t}$). Hence the frequency of the Rabi oscillation is simply proportional to the difference between the overall phases of the two atomic cyclic initial states.

We now turn to the splitting of the Mollow triplet. The joint Hamiltonian H_j has eigenvalues that comprise evenly spaced pairs $(\epsilon_{+,n}, \epsilon_{-,n})$ [Cohen-Tannoudji 1977]. Thus the emission spectrum of the system is a triplet. This is the Mollow triplet [Mollow 1969]. Further, the splitting of the triplet is just the difference $\epsilon_{+,n} - \epsilon_{-,n}$, the Rabi frequency. Thus the overall phases can be interpreted in terms of both the Rabi opscillation and the Mollow triplet. Note that it is the difference in overall phases that can be measured. As discussed in section 3.2, this is because there is only one arbitrary phase in quantum mechanics.

9.2 The Rabi oscillation itself

Having shown how the Berry phases can be interpreted in terms of the Rabi oscillations, I now turn to the Rabi oscillations themselves. As before, the Hamiltonian of the semi-classical Jaynes-Cummings model is given by

$$H = \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix}. \tag{9.13}$$

Consider the arbitrary initial state

$$\phi(0) = \begin{bmatrix} a_+ \\ a_- \end{bmatrix}. \tag{9.14}$$

From equations (5.15) and (5.16), the operators Z and M in the decomposition $U = Z\exp\{\mathrm{i}Mt\}$ are given by

$$Z = \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t} & 0 \\ 0 & 1 \end{bmatrix}, \tag{9.15}$$

$$M = \begin{bmatrix} \frac{\omega}{2} & -k \\ -k & \frac{\omega}{2} \end{bmatrix}. \tag{9.16}$$

As shown in section 5.1, M has eigenvectors (the cyclic initial states)

$$\phi_{\pm}(0) = \sqrt{\tfrac{1}{2}} \begin{bmatrix} \pm 1 \\ 1 \end{bmatrix}, \tag{9.17}$$

with eigenvalues $\frac{\omega}{2} \mp k$. To find the evolved state, we write the initial state in the basis of cyclic initial states:

$$\phi(0) = \sqrt{\tfrac{1}{2}}(a_+ + a_-)\phi_+(0) - \sqrt{\tfrac{1}{2}}(a_+ - a_-)\phi_-(0). \tag{9.18}$$

Thus

$$\begin{aligned} \phi(t) &= U(t)\phi(0) \\ &= \sqrt{\tfrac{1}{2}}(a_+ + a_-)\mathrm{e}^{\mathrm{i}(\omega/2-k)t} Z(t)\phi_+(0) - \sqrt{\tfrac{1}{2}}(a_+ - a_-)\mathrm{e}^{\mathrm{i}(\omega/2+k)t} Z(t)\phi_-(0) \\ &= \tfrac{1}{2}(a_+ + a_-)\mathrm{e}^{\mathrm{i}(\omega/2-k)t} \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t} \\ 1 \end{bmatrix} - \sqrt{\tfrac{1}{2}}(a_+ - a_-)\mathrm{e}^{\mathrm{i}(\omega/2+k)t} \begin{bmatrix} -\mathrm{e}^{-\mathrm{i}\omega t} \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t}(a_+ \cos kt - \mathrm{i}a_- \sin kt) \\ \mathrm{e}^{\mathrm{i}\omega t}(a_- \cos kt - \mathrm{i}a_+ \sin kt) \end{bmatrix}. \end{aligned} \tag{9.19}$$

Hence the probability of finding the system in the upper atomic state is given by

$$\begin{aligned} P_+ &= |a_+ \cos kt - \mathrm{i}a_- \sin kt|^2 \\ &= |a_+|^2 \cos^2 kt + |a_-|^2 \sin^2 kt - \mathrm{i}(\overline{a}_+ a_- - a_+ \overline{a}_-) \cos kt \sin kt \\ &= \tfrac{1}{2}\left(1 + (|a_+|^2 - |a_-|^2)\cos 2kt - \mathrm{i}(a_- \overline{a}_+ - a_+ \overline{a}_-)\sin 2kt\right). \end{aligned} \tag{9.20}$$

This is π/k-periodic, the sinusoidal variation being the Rabi oscillation.

However, substituting $\tilde{t} = \pi/k$ into equation (9.19) gives

$$\phi(\tilde{t}) = - \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\pi\omega/2k} a_+ \\ \mathrm{e}^{\mathrm{i}\pi\omega/2k} a_- \end{bmatrix}, \tag{9.21}$$

which is not periodic (unless $\omega/2k$ is integral or we have taken a_+ or a_- to be zero). Thus the initial state $\phi(0)$ is not cyclic in general. Note that this corrects a small error in Agarwal [1988]. He works in the interaction picture, which effectively means that the troublesome $\exp\{\pm \mathrm{i}\omega t/2\}$ factors are shifted into the operators.

Hence the interaction picture state is cyclic. The problem though is that not all of the observables are cyclic. For example

$$\begin{aligned}\sigma_x^{\mathrm{I}}(t) &= \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t/2} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\omega t/2} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \mathrm{e}^{\mathrm{i}\omega t/2} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\omega t/2} \end{bmatrix} \\ &= \begin{bmatrix} 0 & \mathrm{e}^{-\mathrm{i}\omega t} \\ \mathrm{e}^{\mathrm{i}\omega t} & 0 \end{bmatrix}, \end{aligned} \tag{9.22}$$

and so is not cyclic. Thus to claim that the system is cyclic when the interaction picture state is cyclic is misleading. In fact one could follow the logic further and look at the Heisenberg picture state. As this is time-independent, one would be tempted to say that all initial states are cyclic! Despite this subtlety, the interaction picture is useful to see why the Rabi oscillations occur. This is because the interaction picture inversion operator $\sigma_z^{\mathrm{I}}(t)$ is cyclic.

Of course one could still, in principle, calculate the Berry phases in the interaction (or any other) picture. The problem is that then one must be very careful to evaluate the geometric contributions from both the time dependence of the state and the time dependence of the operators. In general, the easiest way to do this is to move all of the time dependence into the states, that is to transform into the Schrödinger picture. One notable exception is Salzman's decomposition, which was treated in section 5.3. For the special cases that it can be used for, all of the geometric information about the time evolution is maintained in the interaction picture states. Thus for this special case, calculations can be done transparently in either the interaction or Schrödinger picture.

Even though the initial state is not cyclic, we can still discuss the evolution of its overall phase. To do this we need to extend the definition of the overall phase to the case when the initial state is not cyclic. We define the Pancharatnam phase difference between the two non-orthogonal vectors ψ_1 and ψ_2 as the phase of $\langle \psi_1 \mid \psi_2 \rangle$. This obviously reduces to the usual phase difference when ψ_1 and ψ_2 are on the same ray in Hilbert space (are equal up to a phase) [Berry 1987]. This definition is motivated by the interference of light beams. Those beams that are in phase should constructively interfere and those that are out of phase should destructively interfere. However it does not make the overall phase an observable

in the sense of being represented by a self-adjoint operator. This is discussed more fully in section 11.2.

To find the overall phase we must evaluate $\langle\phi(0) \mid \phi(\tilde{t})\rangle$. We have

$$\begin{aligned}\langle\phi(0) \mid \phi(\tilde{t})\rangle &= [\overline{a}_+, \overline{a}_-] \begin{bmatrix} -\mathrm{e}^{-\mathrm{i}\pi\omega/2k} a_+ \\ -\mathrm{e}^{\mathrm{i}\pi\omega/2k} a_- \end{bmatrix} \\ &= -\left(\cos\frac{\pi\omega}{2k} - \mathrm{i}\sin\frac{\pi\omega}{2k}\right)|a_+|^2 - \left(\cos\frac{\pi\omega}{2k} + \mathrm{i}\sin\frac{\pi\omega}{2k}\right)|a_-|^2 \\ &= -\left(\cos\frac{\pi\omega}{2k} - \mathrm{i}\sin\frac{\pi\omega}{2k}(|a_+|^2 - |a_-|^2)\right). \end{aligned} \tag{9.23}$$

Setting this equal to $r\exp\{\mathrm{i}\chi\}$, we can see that the overall phase is given by $\chi = \pi + \alpha$, where

$$\tan\alpha = -(|a_+|^2 - |a_-|^2)\tan\frac{\pi\omega}{2k}. \tag{9.24}$$

To find the Berry phases, we need the dynamical phases (the single-valued vector formalism cannot be used as the initial states are not truly periodic). We have

$$\begin{aligned} H\phi(t) &= \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix} \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t/2}(a_+\cos kt - \mathrm{i}a_-\sin kt) \\ \mathrm{e}^{\mathrm{i}\omega t/2}(a_-\cos kt - \mathrm{i}a_+\sin kt) \end{bmatrix} \\ &= \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t/2}\left(\left(\frac{\omega}{2}a_+ + ka_-\right)\cos kt - \mathrm{i}\left(\frac{\omega}{2}a_- + ka_+\right)\sin kt\right) \\ \mathrm{e}^{\mathrm{i}\omega t/2}\left(\left(-\frac{\omega}{2}a_- + ka_+\right)\cos kt - \mathrm{i}\left(-\frac{\omega}{2}a_+ + ka_-\right)\sin kt\right) \end{bmatrix}. \end{aligned} \tag{9.25}$$

This gives

$$\begin{aligned}\langle\phi(t) \mid H \mid \phi(t)\rangle &= \cos^2 kt\left(\overline{a}_+(\tfrac{\omega}{2}a_+ + ka_-) + \overline{a}_-(-\tfrac{\omega}{2}a_- + ka_+)\right) \\ &\quad + \sin^2 kt\left(\overline{a}_-(\tfrac{\omega}{2}a_- + ka_+) + \overline{a}_+(-\tfrac{\omega}{2}a_+ + ka_-)\right) \\ &= \tfrac{\omega}{2}(|a_+|^2 - |a_-|^2)\cos 2kt + \tfrac{\mathrm{i}\omega}{2}(\overline{a}_-a_+ - \overline{a}_+a_-)\sin 2kt \\ &\quad + k(\overline{a}_+a_- + \overline{a}_-a_+). \end{aligned} \tag{9.26}$$

Now $\int_0^{\pi/k}\sin 2kt\,\mathrm{d}t$ and $\int_0^{\pi/k}\cos 2kt\,\mathrm{d}t$ are both zero. Hence the dynamical phase is given by

$$\begin{aligned}\delta &= -\int_0^{\pi/k}\langle\phi(t) \mid H \mid \phi(t)\rangle\,\mathrm{d}t \\ &= -\pi(\overline{a}_+a_- + \overline{a}_-a_+). \end{aligned} \tag{9.27}$$

We are now in a position to calculate the Berry phases for the problem. We have that

$$\gamma = \pi(1 + \overline{a}_+ a_- + \overline{a}_- a_+) + \alpha. \tag{9.28}$$

Note that if $a_+ = 0$ or $a_- = 0$ the dynamical phase vanishes and we have $\alpha = \mp\pi\omega/2k$ so that $\gamma = \pi(1 \mp \pi\omega/2k)$ in agreement with Agarwal [1988].

Having discussed the semi-classical Jaynes-Cummings model, I now turn to the fully quantum mechanical case. We find that we get Rabi oscillations and cyclic behaviour for initial states in the space spanned by $\{|+,n\rangle, |-,n+1\rangle\}$, but that the Rabi oscillations for the initial states closest to the semi-classical ones collapse and revive due to the granular nature of the field.

As the joint electron-photon Hamiltonian

$$H_j = \tfrac{\omega}{2}\sigma_z + \omega b^* b + \lambda(\sigma_+ b + \sigma_- b^*) \tag{9.29}$$

is time-independent, it is convenient to invoke the concept of quasi-degeneracy discussed in section 5.2. To recapitulate, two cyclic initial states $\phi_1(0)$ and $\phi_2(0)$ are quasi-degenerate if they have the same overall phase. In this case, any linear combination of them is also a cyclic initial state with the same overall phase.

Now, barring quasi-degeneracy, the cyclic initial states of a time-independent Hamiltonian are precisely the eigenvectors of the Hamiltonian. But, as the dynamical phase is defined with reference to time-independent systems, all of these states have a Berry phase of zero. The only way to get a non-trivial Berry phase for time-independent systems is to take a linear combination of two quasi-degenerate eigenvectors with different eigenvalues. This will not in general be an eigenvector of the Hamiltonian and so is not prohibited from having a non-zero Berry phase.

By direct substitution, one can easily verify that the eigenvectors and eigenvalues of the Hamiltonian (9.29) are

$$|\,\epsilon_{\alpha n}\rangle = \pm\sqrt{\tfrac{1}{2}}\,|+,n\rangle + \sqrt{\tfrac{1}{2}}\,|-,n+1\rangle, \tag{9.30}$$

$$\epsilon_{\alpha n} = (n + \tfrac{1}{2})\omega \pm \lambda\sqrt{n+1}. \tag{9.31}$$

For convenience, we ignore the ground state $\mid \epsilon_g\rangle$ which has energy $\epsilon_g = -\frac{\omega}{2}$. If we put $\tilde{t} = \pi(\lambda\sqrt{n+1})^{-1}$ then the two states $\mid \epsilon_{\pm,n}\rangle$ become quasi-degenerate. Hence any linear combination of these two states is a cyclic initial state (for the period $\tilde{t}$). As the two eigenvectors are formed from $\mid +,n\rangle$ and $\mid -,n+1\rangle$, these cyclic initial states are in fact in the space spanned by $\{\mid +,n\rangle, \mid -,n+1\rangle\}$. To get the overall phase we need merely evaluate $\epsilon_{-n}\tilde{t}$. We have

$$\begin{aligned}\chi &= -\epsilon_{-n}\tilde{t} \\ &= -\pi\frac{(n+\frac{1}{2})\omega - \lambda\sqrt{n+1}}{\lambda\sqrt{n+1}} \\ &= \pi - \frac{(n+\frac{1}{2})\omega\pi\omega}{\lambda\sqrt{n+1}}.\end{aligned} \tag{9.32}$$

This cyclic evolution gives rise to Rabi oscillations as in the semi-classical case, except now the states are themselves cyclic. To find the Berry phases we need merely apply equation (6.17). Hence the cyclic initial state $\phi(0) = a_+ \mid +,n\rangle + a_- \mid -,n+1\rangle$ has Berry phase $\gamma = 2\pi|a_+|^2$.

This result contrasts with the semi-classical result discussed earlier. There we got Rabi oscillations but the initial states were not cyclic. However, to compare the two cases properly, we should start in the product of a photon coherent state and an arbitrary electronic state. But when we do this we find that we no longer get perfect Rabi oscillations. Instead there are collapses and revivals in the probability of finding the system in the upper state [Knight 1986]. This is related to the fact that the coherent state contains contributions from all photon numbers, and we cannot find a period that makes all of the eigenvalues $\epsilon_{\pm n}$ quasi-degenerate.

Now if the collapses and revivals were themselves perfect, we could analyse them in terms of Berry (or Pancharatnam) phases. However they are not, a fact that can be traced back to the appearance of the factor $\sqrt{n+1}$ in expression (9.31). As I will now show, if they had involved $n+1$ instead of $\sqrt{n+1}$, then the revivals would have been exact. To do this I will discuss the quantum optical system consisting of two degenerate atomic levels coupled through a virtual level by a Raman transisition [Phoenix and Knight 1990]. The same analysis holds for the two-level atom with intensity dependent coupling [Bužek and Jex 1990].

The system has Hamiltonian

$$H = \omega b^* b + \lambda b^* b(\sigma_+ + \sigma_-). \tag{9.33}$$

We will see that for initial coherent states, the collapses and revivals seen in the quantum Jaynes-Cummings model are now perfect. However, as was the case with the semi-classical Rabi oscillations, the states are not cyclic and we must use the concept of Pancharatnam phase.

We proceed as before. H has eigenvectors and eigenvalues

$$\mid \epsilon_{\alpha n} = \sqrt{\tfrac{1}{2}} \mid +, n\rangle \pm \sqrt{\tfrac{1}{2}} \mid -, n\rangle, \tag{9.34}$$

$$\epsilon_{\alpha n} = n(\omega \pm \lambda). \tag{9.35}$$

Thus the energy involves n instead of $\sqrt{n}$. Taking $\tilde{t} = \pi/n\lambda$ gives Rabi oscillations as before. Interestingly we can also get other quasi-degeneracy effects. If we take $\tilde{t} = 2\pi/(\omega + \lambda)$ then all of the $\mid \epsilon_{+,n}\rangle$ are quasi-degenerate, while if we take $\tilde{t} = \pi/(\omega - \lambda)$ then all of the $\mid \epsilon_{-,n}\rangle$ are quasi-degenerate.

However, we are most interested in the behaviour of a system initially in the direct product of a photon coherent state and an electronic state. Let the initial state be

$$\phi(0) = \mid z\rangle(a_+ \mid +\rangle + a_- \mid -\rangle), \tag{9.36}$$

where the coherent state $\mid z\rangle$ is given by

$$\mid z\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n\,!}} \mid n\rangle. \tag{9.37}$$

To find the evolved state we decompose the state (9.36) in the set of eigenvectors. We have

$$\phi(0) = \sum_{n=0}^{\infty} \sqrt{\tfrac{1}{2}} \mathrm{e}^{-|z|^2} \frac{z^n}{\sqrt{n\,!}} \left((a_+ + a_-) \mid \epsilon_{+,n}\rangle + (a_+ - a_-) \mid \epsilon_{,n}\rangle \right). \tag{9.38}$$

Thus

$$\begin{aligned}\phi(t) = \sum_{n=0}^{\infty} \sqrt{\tfrac{1}{2}} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \big(& (a_+ + a_-)\mathrm{e}^{-\mathrm{i}n\omega t}\mathrm{e}^{-\mathrm{i}n\lambda t} \mid \epsilon_{+,n}\rangle \\ & + (a_+ - a_-)\mathrm{e}^{-\mathrm{i}n\omega t}\mathrm{e}^{\mathrm{i}n\lambda t} \mid \epsilon_{-,n}\big) \\ = \sum_{n=0}^{\infty} \tfrac{1}{2} \mathrm{e}^{-|z|^2/2} \frac{(z\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}} \big(& \big((a_+ + a_-)\mathrm{e}^{-\mathrm{i}n\lambda t} + (a_+ - a_-)\mathrm{e}^{\mathrm{i}n\lambda t}\big) \mid +, n\rangle \\ & \big((a_+ + a_-)\mathrm{e}^{-\mathrm{i}n\lambda t} - (a_+ - a_-)\mathrm{e}^{\mathrm{i}n\lambda t}\big) \mid -, n\rangle\big) \\ = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{(z\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}} \big(& (a_+ \cos n\lambda t - \mathrm{i}a_- \sin n\lambda t) \mid +, n\rangle \\ & + (a_- \cos n\lambda t - \mathrm{i}a_+ \sin n\lambda t) \mid -, n\rangle\big). \end{aligned} \tag{9.39}$$

Now let $\tilde{t} = 2\pi/\lambda$. Substituting into equation (9.39), the final state is given by

$$\begin{aligned}\phi(\tilde{t}) &= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{(z\mathrm{e}^{-\mathrm{i}\omega\tilde{t}})^n}{\sqrt{n!}} (a_+ \mid +, n\rangle + a_- \mid -, n\rangle) \\ &= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{(z\mathrm{e}^{-\mathrm{i}\omega\tilde{t}})^n}{\sqrt{n!}} \mid n\rangle \quad (a_+ \mid +\rangle + a_- \mid -\rangle) \\ &= \mid z\mathrm{e}^{-\mathrm{i}\omega\tilde{t}}\rangle (a_+ \mid +\rangle + a_- \mid -\rangle). \end{aligned} \tag{9.40}$$

Thus the probability of finding the system in the upper state is $2\pi/\lambda$-periodic, that is we have exact collapses and revivals.

Now, no two distinct coherent states are equal up to a phase. Hence, unless $\omega\tilde{t}$ is an integral multiple of 2π, the general initial state is not cyclic. Thus, as with the semi-classical case, to compare the phases of the initial and final states we must use the Pancharatnam phase. In section B.1 I show that the inner product of two coherent states $\mid v\rangle$ and $\mid v'\rangle$ is given by

$$\langle v \mid v'\rangle = \exp\{-|v|^2/2 - |v'|^2/2 + v\overline{v}'\}. \tag{9.41}$$

Thus the inner product of the initial and final states is given by

$$\begin{aligned}\langle \phi(0) \mid \phi(\tilde{t})\rangle &= \langle z \mid z\mathrm{e}^{-\mathrm{i}\omega t}\rangle \\ &= \mathrm{e}^{-|z|^2/2}\mathrm{e}^{-|z|^2/2}\mathrm{e}^{|z|^2\exp\{-\mathrm{i}\omega\tilde{t}\}}\end{aligned}$$

$$
\begin{aligned}
&= \exp\{|z|^2(-1+\mathrm{e}^{-\mathrm{i}\omega\tilde{t}})\} \\
&= \exp\{|z|^2(-1+\cos\omega\tilde{t})\}\exp\{-\mathrm{i}|z|^2\sin\omega\tilde{t}\} \\
&= \exp\{-2|z|^2\sin^2(\omega\tilde{t}/2)\}\exp\{-\mathrm{i}|z|^2\sin\omega\tilde{t}\}, \qquad (9.42)
\end{aligned}
$$

giving the overall phase $\chi = -|z|^2\sin\omega\tilde{t}$.

We now need the dynamical phase. From equation (9.39) we have

$$
\begin{aligned}
\phi(t) &= \sum_{n=0}^{\infty}\mathrm{e}^{-|z|^2/2}\frac{(z\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}}\big((a_+\cos n\lambda t - \mathrm{i}a_-\sin n\lambda t)\mid +,n\rangle \\
&\qquad + (a_-\cos n\lambda t - \mathrm{i}a_+\sin n\lambda t)\mid -,n\rangle\big) \\
&= \sum_{n=0}^{\infty}\sqrt{\tfrac{1}{2}}\mathrm{e}^{-|z|^2/2}\frac{(z\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}}\big((a_+ + a_-)\mathrm{e}^{-\mathrm{i}n\lambda t}\mid \epsilon_{+,n}\rangle \\
&\qquad + (a_+ - a_-)\mathrm{e}^{\mathrm{i}n\lambda t}\mid \epsilon_{-,n}\rangle\big) \\
\Rightarrow\ H\phi(t) &= \sqrt{\tfrac{1}{2}}\mathrm{e}^{-|z|^2/2}\frac{(z\mathrm{e}^{-\mathrm{i}\omega t})^n}{\sqrt{n!}}\big((a_+ + a_-)\mathrm{e}^{-\mathrm{i}n\lambda t}n(\omega+\lambda)\mid \epsilon_{+,n}\rangle \\
&\qquad + (a_+ - a_-)\mathrm{e}^{\mathrm{i}n\lambda t}n(\omega-\lambda)\mid \epsilon_{-,n}\rangle\big). \qquad (9.43)
\end{aligned}
$$

Hence we have

$$
\begin{aligned}
\langle\phi(t)\mid H(t)\mid\phi(t)\rangle &= \sum_{n=0}^{\infty}\tfrac{1}{2}\mathrm{e}^{-|z|^2}\frac{|z|^2n}{n!}\big((\overline{a}_+ + \overline{a}_-)(a_+ + a_-)n(\omega+\lambda) \\
&\qquad + (\overline{a}_+ - \overline{a}_-)(a_+ - a_-)n(\omega-\lambda)\big) \\
&= |z|^2\left(\omega + \lambda(\overline{a}_+a_- + a_+\overline{a}_-)\right) \\
\Rightarrow\qquad \delta &= -\int_0^{\tilde{t}}\langle\phi(t)\mid H(t)\mid\phi(t)\rangle\,\mathrm{d}t \\
&= -2\pi|z|^2\left(\frac{\omega}{\lambda} + \overline{a}_+a_- + a_+\overline{a}_-\right). \qquad (9.44)
\end{aligned}
$$

We can now find the Berry phase. Using the fact that $\gamma = \chi - \delta$, we immediately have that

$$
\gamma = |z|^2\left(-\sin\frac{2\pi\omega}{\lambda} + 2\pi\left(\frac{\omega}{\lambda} + \overline{a}_+a_- + a_+\overline{a}_-\right)\right). \qquad (9.45)
$$

Note that Phoenix and Knight [1990] find that the field state is cyclic. However they work in the interaction picture and, as I have discussed previously in connection with Agarwal's work, cyclicity in the interaction picture is not a true measure of periodicity.

9.3 Extensions

The analysis of the preceeding sections can be usefully extended in many ways. For example, the effects of spontaneous emission have been ignored. In this section I will comment on some of the more important generalisations. In section 9.1 I demonstrated how the overall phase in a fermion subsystem coupled to a single boson mode can be interpreted in terms of the energy levels of the time-independent joint system. This can be generalised to include either more than one boson mode or anharmonicity. I discuss systems with degenerate boson modes first.

Given a constant boson-fermion Hamiltonian with N degenerate boson modes we can form the semi-classical fermion Hamiltonian by replacing the N creation operators b_j^* with the functions $\exp\{\mathrm{i}\theta_j\}\exp\{\mathrm{i}\omega t\}$. This gives the same result as if we had taken the semi-classical limit of the single-mode Hamiltonian that arises when we replace the creation operator b_j^* with the rephased operator $\exp\{\mathrm{i}\theta_j\}b^*$. For example, take the D_4 Jahn-Teller Hamiltonian

$$H = E1 + \omega(b_1^* b_1 + b_2^* b_2) + \lambda\left(-\sigma_y(b_1^* + b_1) + \sigma_x(b_2^* + b_2)\right) \tag{9.46}$$

discussed by Moore and Stedman [1990a]. This system was discussed in section 4.2. H has the same semi-classical limit, and so the same Berry phases, as the single mode Hamiltonian

$$H' = E1 + \omega a^* a + 2\lambda \sin^{1/2}\zeta\left(\sigma_+ a^* + \sigma_- a\right). \tag{9.47}$$

This involves the squeezed mode [Yuen 1976]

$$a = \mu b + \nu b^*, \tag{9.48}$$

where $\mu = (2\sin^{1/2}\zeta)^{-1}(1 + \mathrm{i}\exp\{-\mathrm{i}\zeta\})$, $\nu = (2\sin^{1/2}\zeta)^{-1}(1 + \mathrm{i}\exp\{\mathrm{i}\zeta\})$ and we have replaced the two phonon creation operators b_1^* and b_2^* with b^* and $\exp\{\mathrm{i}\zeta\}b^*$ respectively.

We can also analyse boson-fermion Hamiltonians involving anharmonicity. Consider a general $\tilde{t}$-periodic fermionic Hamiltonian H with Fourier decompositon

$$H = \sum_{n=-\infty}^{\infty} H^{[n]} \mathrm{e}^{\mathrm{i}n\omega t}. \tag{9.49}$$

Then, if we make the replacement

$$e^{in\omega t} = \begin{cases} b^{*n} & : n \geq 0 \\ b^n & : n < 0 \end{cases}, \tag{9.50}$$

we generate a constant boson-fermion Hamiltonian that gives H in the semi-classical limit. Note that the Fourier components with $|n| > 1$ give anharmonicity. Thus we can interpret the overall phases of any periodic fermionic system in terms of the energy levels of a certain time-independent boson-fermion Hamiltonian. These two examples are taken from Moore [1990b].

The analysis can also be extended in other ways. For example, we can superimpose an adiabatic variation of the laser parameters (such as the detuning and laser phase) onto the non-adiabatically periodic system [Moore and Stedman 1990c, Barnett *et al.* 1988]. This will be discussed further in the next chapter. One can also start in a non-classical state of the radiation field. For instance, Mahran and Obada [1988] analyse the logarithmic state and Colegrave and Ramjit [1989] a state with few photons. These cases will not be discussed further.

The last two generalisations I will discuss involve two of the important assumptions made in the Jaynes-Cummings model, namely the use of the rotating wave approximation and the neglect of spontaneous emission. First the rotating wave approximation.

The interaction Hamiltonian of a linearly polarised laser and a two-level atom has the electric dipole form

$$V = (\sigma_+ + \sigma_-)(b^* + b). \tag{9.51}$$

In the rotating wave approximation the "counter-rotating" terms $\sigma_+ b^* + \sigma_- b$ are ignored as they are strongly non-energy conserving [Cohen-Tannoudji 1977]. However the counter-rotating terms do have a measurable effect, the most well-known manifestation of which is the Bloch-Siegert shift [Bloch and Siegert 1940]. It has also been noted that the introduction of non-rotating wave terms can lead to the onset of chaos [Milonni *et al.* 1983].

The usual approach to the calculation of non-rotating wave effects is by perturbation theory [Phoenix 1989, Silverman and Pipkin 1972]. This method is crucially important for the analysis of Moore and Stedman [1990c] presented in the next chapter. By varying the laser phase, they generate an adiabatic Berry phase which adds to the non-adiabatic Berry phase that is present even if the phase is not varied. Their path goes through a point where the rotating wave eigenfunctions are degenerate. Thus on the face of it the adiabatic theorem should not hold. However, the non-rotating wave perturbation lifts the degeneracy, making the adiabatic theorem applicable.

Another method of dealing with counter-rotating terms has been found recently. For restricted values of the detuning and coupling constant, exact solutions can be expressed in terms of the elliptic Jacobian functions [Jeleńska-Kuklińska and Kuś 1990]. This approach is based on the work of Judd [1979] on the Jahn-Teller effect.

Finally, the effects of spontaneous emission can be easily included. The semi-classical Hamiltonian is perturbed by a phenomenological non-self-adjoint operator which models the loss in the system [Stenholm 1973]. This means that the evolution is no longer unitary and so the norm of $\|\phi(t)\|$ of the evolving state decays with time. However, this implies that no initial state can be cyclic in the standard sense. To handle this problem, we generalise our definitions. Assuming that the initial state is normalised, an initial state is called cyclic (with overall phase χ) if $\phi(\tilde{t}) = r\exp\{\mathrm{i}\chi\}\phi(0)$, where $r = \|\phi(\tilde{t})\|$. To find the Berry phases we need the generalised single-valued vectors. Clearly these are just the vectors $\psi(t) = \exp\{\mathrm{i}\theta(t)\}\phi(t)$ with $\psi(\tilde{t}) = r\psi(0)$ (or equivalently $\theta(\tilde{t}) = \chi$). Then, by the analysis leading to equation (3.8), the Berry phase is given by

$$\gamma = \mathrm{i}\int_0^{\tilde{t}} \langle\psi(t) \mid \dot{\psi}(t)\rangle \,\mathrm{d}t. \tag{9.52}$$

This agrees with Chu *et al.* [1989] and Garrison and Wright [1988]. The dissipative problem has also been analysed by Gamliel and Freed [1989] in the adiabatic context.

Chapter Ten

Adiabatic variation

Until now, the time-dependence of the Hamiltonians we have been studying has been either purely adiabatic or purely non-adiabatic. In this chapter I consider what happens when the two are superimposed. That is, an adiabatic time-variation is imposed onto an already non-adiabatically periodic Hamiltonian. A good example of this is a two-level atom in a semi-classical radiation field, where we adiabatically vary the laser parameters (such as the phase and polarisation).

Consider a non-adiabatic Hamiltonian $H(\mathbf{R},t)$ that depends on some parameter $\mathbf{R}$. For fixed $\mathbf{R}$, we assume that $H(\mathbf{R},t)$ is $\tilde{t}_N$-periodic. Now vary $\mathbf{R}$ adiabatically around some closed path with period $\tilde{t}_A$: $R(\tilde{t}_A) = R(0)$. For the resulting mixed Hamiltonian to be $\tilde{t}_A$-periodic, we require that $\tilde{t}_A = N\tilde{t}_N$. That is, there must be an integral number of non-adiabatic periods in each adiabatic period. For the variation of $\tilde{t}_A$ to be adiabatic, $\tilde{t}_A$ must be large, which is equivalent to requiring that N be large. Further, as $\mathbf{R}$ is varied smoothly, $\mathbf{R}$ does not change much from time $t = n\tilde{t}$ to $t = (n+1)\tilde{t}$. This fact will be very useful when we come to split the Berry phase into the sum of its adiabatic and non-adiabatic parts.

The result of this mixing can be rationalised very simply. When we made the transition from a time-independent Hamiltonian to a non-adiabatic Hamiltonian, the position of the Hamiltonian eigenvectors as the "stationary states" was supplanted by the cyclic initial states. Further, in the transition from a time-independent Hamiltonian to an adiabatic Hamiltonian, the eigenstates were replaced by the instantaneous eigenvectors. Thus, it should come as no surprise that in the transition from adiabatic to adiabatic superimposed with non-adiabatic

evolution, the cyclic initial states are merely replaced by the instantaneous cyclic initial states. That is, the cyclic initial states of the mixed Hamiltonian $H(\mathbf{R}(t), t)$ are just the cyclic initial states of the non-adiabatic Hamiltonian $H(\mathbf{R}(0), t)$.

Now, due to the non-adiabatic time dependence, we cannot use the normal adiabatic theorem to find the Berry phases. Hence we need a modified ansatz. In sections 10.1 and 10.2, I will derive this ansatz in two different ways. The first is due to Moore and Stedman [1990c]. They give a heuristic argument based on a simple model problem, the semi-classical Jaynes-Cummings model with varying laser phase. This system is exactly solvable due to the relationship between the semi-classical Hamiltonian and the parent quantum Hamiltonian, which is a normal adiabatic system. Using this formalism, we find that the Berry phase splits into the sum of two parts. The first is the sum of a non-adiabatic Berry phase for each of the many non-adiabatic periods $\tilde{t}_N$ that go into the single adiabatic period $\tilde{t}_A$. The second is an adiabatic Berry phase due to global twisting [Liang 1989].

The second approach is due to Breuer *et al.* [1990]. They use the fact that the system has two separate time scales, $\tilde{t}_N$ and $\tilde{t}_A$. The modified adiabatic ansatz can then be found by using two separate time parameters, one for each scale. This method ties the mixed problem to the Fourier analysis of section 6.1, and makes clear the limitations of the theory due to narrowly avoided crossings.

Finally, in section 10.3 I discuss an example, the two-level atom in a laser with varying polarisation. We include both the rotating wave and non-rotating wave couplings. The variation of the polarisation amounts to a variation of the two coupling coefficients. That this must be so is most easily seen on symmetry grounds. Consider an electronic transition between an s state and a p_{-1} state split from the other p states by, say, a magnetic field. Then for certain polarisations the rotating wave (or non-rotating wave) transisition will be forbidden, making the effective coupling constant zero.

10.1 Moore and Stedman's result

The Hamiltonians we are considering have both adiabatic and non-adiabatic time dependences and so the normal adiabatic theorem cannot be used. In this section, the problem is solved by analogy with a simple solvable problem. This approach was first used by Moore and Stedman [1990c]. In the next section, a two-time approach due to Breuer *et al.* [1990] is used. We note that Ellinas *et al.* [1989] have also discussed this problem, using the eigenmatrices of the Liouvillian superoperator.

Consider the Hamiltonian

$$H(t) = \begin{bmatrix} \frac{\omega}{2} & k\mathrm{e}^{-\mathrm{i}\theta(t)}\mathrm{e}^{-\mathrm{i}\omega t} \\ k\mathrm{e}^{\mathrm{i}\theta(t)}\mathrm{e}^{\mathrm{i}\omega t} & -\frac{\omega}{2} \end{bmatrix}, \tag{10.1}$$

where $\theta(t)$ is an adiabatic parameter satisfying $\theta(0) = 0$, $\theta(\tilde{t}_A) = 2\pi$. This arises when the phase of a semi-classical radiation field, which is incident upon a two-level atom, is varied. By the same argument as in section 2.2, this can be shown to arise as the semi-classical limit of the purely adiabatic quantum Hamiltonian

$$H_j = \tfrac{\omega}{2}\sigma_z + \omega b^* b + \lambda\left(\mathrm{e}^{-\mathrm{i}\theta(t)}\sigma_+ b + \mathrm{e}^{\mathrm{i}\theta(t)}\sigma_- b^*\right), \tag{10.2}$$

where the initial state is the product of an electronic state $\phi(0)$ and a photon coherent state $\mid z\rangle$ and $k = \lambda z$. The only difference in the proof is that the Hamiltonian (10.2) is adiabatic, not time-independent, and so the adiabatic theorem must be used.

Let the initial electronic state be

$$\phi(0) = a_+ \mid +\rangle + a_- \mid -\rangle. \tag{10.3}$$

Then, from the proof of equation (2.17), the density operator $\rho(0) = \mid \phi(0)\rangle\langle\phi(0) \mid$ evolves into $\rho(t) = \mid \tilde{\psi}(t)\rangle\langle\tilde{\psi}(t) \mid$, where

$$\begin{aligned}\tilde{\psi}(t) = \tfrac{1}{2}\mathrm{e}^{-\mathrm{i}\theta(t)}\mathrm{e}^{-\mathrm{i}\omega t}\left((a_+ + a_-)\mathrm{e}^{-\mathrm{i}kt} + (a_+ - a_-)\mathrm{e}^{\mathrm{i}kt}\right) \mid +\rangle \\ + \tfrac{1}{2}\left((a_+ + a_-)\mathrm{e}^{-\mathrm{i}kt} - (a_+ - a_-)\mathrm{e}^{\mathrm{i}kt}\right) \mid -\rangle.\end{aligned} \tag{10.4}$$

Thus $\phi(0)$ evolves into $\tilde{\psi}(t)$ up to a phase. The fact that the phase is not known is not important, as all we will require is a single-valued vector.

Now the adiabatic period $\tilde{t}_A$ is an integral multiple of the non-adiabatic period $2\pi/\omega$. Thus $\exp\{-\mathrm{i}\omega\tilde{t}_A\} = 1$. Similarly, as we take the parameters around a closed path, $\exp\{-\mathrm{i}\theta(\tilde{t}_A)\}$ is also unity. Therefore substituting $t = \tilde{t}_A$ into equation (10.4) gives

$$\begin{aligned}\tilde{\psi}(\tilde{t}_A) = \tfrac{1}{2}\left((a_+ + a_-)\mathrm{e}^{-\mathrm{i}k\tilde{t}_A} + (a_+ - a_-)\mathrm{e}^{\mathrm{i}k\tilde{t}_A}\right) \mid +\rangle \\ + \tfrac{1}{2}\left((a_+ + a_-)\mathrm{e}^{-\mathrm{i}k\tilde{t}_A} - (a_+ - a_-)\mathrm{e}^{\mathrm{i}k\tilde{t}_A}\right) \mid -\rangle. \qquad (10.5)\end{aligned}$$

For $\phi(0)$ to be a cyclic initial state, it is plainly necessary and sufficient that $\tilde{\psi}(t)$ return to itself up to a phase. Try $a_+ = \pm\sqrt{\frac{1}{2}}$ and $a_- = \sqrt{\frac{1}{2}}$. Then

$$\begin{aligned}\tilde{\psi}(\tilde{t}_A) &= \pm\sqrt{\tfrac{1}{2}}(\cos k\tilde{t}_A \mp \mathrm{i}\sin k\tilde{t}_A) \mid +\rangle + \sqrt{\tfrac{1}{2}}(\cos k\tilde{t}_A \mp \mathrm{i}\sin k\tilde{t}_A) \mid -\rangle \\ &= \mathrm{e}^{\mp\mathrm{i}k\tilde{t}_A}\tilde{\psi}(0). \qquad (10.6)\end{aligned}$$

Hence the cyclic initial states are given by

$$\phi(0) = \sqrt{\tfrac{1}{2}}\begin{bmatrix}\pm 1\\ 1\end{bmatrix}. \qquad (10.7)$$

To get the Berry phases we need a single valued vector. Using the fact that

$$\tilde{\psi}(t) = \sqrt{\tfrac{1}{2}}\mathrm{e}^{\mp\mathrm{i}kt}\begin{bmatrix}\pm\mathrm{e}^{-\mathrm{i}\theta(t)}\mathrm{e}^{-\mathrm{i}\omega t}\\ 1\end{bmatrix}, \qquad (10.8)$$

the single valued vectors are clearly given by

$$\psi_\pm(t) = \sqrt{\tfrac{1}{2}}\begin{bmatrix}\pm\mathrm{e}^{-\mathrm{i}\theta(t)}\mathrm{e}^{-\mathrm{i}\omega t}\\ 1\end{bmatrix}. \qquad (10.9)$$

Thus, noting that $\omega = 2\pi/\tilde{t}_N = 2N\pi/\tilde{t}_A$, the Berry phases are given by

$$\begin{aligned}\gamma_\pm &= \mathrm{i}\int_0^{\tilde{t}_A}\langle\psi_\pm \mid \dot{\psi}_\pm\rangle\,\mathrm{d}t \\ &= \tfrac{\mathrm{i}}{2}\int_0^{\tilde{t}}(-\mathrm{i}\dot{\theta} - \mathrm{i}\omega)\,\mathrm{d}t \\ &= \tfrac{1}{2}[\theta + \omega t]_0^{\tilde{t}} \\ &= (N+1)\pi. \qquad (10.10)\end{aligned}$$

We now wish to split the Berry phase (10.10) into its adiabatic and non-adiabatic components. To get the adiabatic component we note that the quantum Hamiltonian (10.2) is purely adiabatic. Thus we can apply the formalism of section 4.2. $H_j(t)$ has instantaneous eigenvectors

$$| \epsilon_{\pm,n} \rangle = \pm\sqrt{\tfrac{1}{2}}\mathrm{e}^{-\mathrm{i}\theta(t)} \mid +, n-1\rangle + \sqrt{\tfrac{1}{2}} \mid -, n\rangle. \tag{10.11}$$

As these are single-valued, we need merely substitute into equation (3.8), giving

$$\begin{aligned} \Gamma^A_{\pm} &= \mathrm{i}\int_0^{\tilde{t}_A} \langle \epsilon_{\pm,n} \mid \dot{\epsilon}_{\pm,n} \rangle \, \mathrm{d}t \\ &= \pi. \end{aligned} \tag{10.12}$$

This is essentially the approach taken by Andreev *et al.* [1990].

For the non-adiabatic contribution we consider the Hamiltonian (10.1), but now with θ a fixed parameter. This is a normal non-adiabatic $2\pi/\omega$-periodic Hamiltonian. The evolution operator decomposition of equation (5.8) can easily be shown to be

$$Z = \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\omega t} & 0 \\ 0 & 1 \end{bmatrix}, \tag{10.13}$$

$$M = \begin{bmatrix} \frac{\omega}{2} & -k\mathrm{e}^{-\mathrm{i}\theta} \\ -k\mathrm{e}^{\mathrm{i}\theta} & \frac{\omega}{2} \end{bmatrix}. \tag{10.14}$$

Thus the non-adiabatic cyclic initial states (the eigenvectors of M) are

$$\phi^{\theta}_{\pm}(0) = \sqrt{\tfrac{1}{2}} \begin{bmatrix} \pm\mathrm{e}^{-\mathrm{i}\theta} \\ 1 \end{bmatrix}, \tag{10.15}$$

with Berry phases

$$\begin{aligned} \gamma^{\theta}_{\pm} &= \mathrm{i}\int_0^{\tilde{t}} \langle \phi^{\theta}_{\pm}(0) \mid Z^* \dot{Z} \mid \phi^{\theta}_{\pm}(0) \rangle \, \mathrm{d}t \\ &= \pi. \end{aligned} \tag{10.16}$$

Two points can now be made. The first is that the Berry phase is just the sum of a non-adiabatic Berry phase for each of the N non-adiabatic periods that go into a single adiabatic period and a single adiabatic contribution. Second,

the cyclic initial states are just the non-adiabatic cyclic initial states of $H(\theta(0))$. Further, the single-valued vectors $\psi(t)$ are the single-valued vectors of $H(\theta(t))$ taken at time t. As I will now show, this gives our modified ansatz.

Consider an arbitrary $\tilde{t}_N$ periodic Hamiltonian $H(\mathbf{R},t)$ depending parametrically upon $\mathbf{R}$. In the example above, $\mathbf{R}$ was the laser phase. For constant $\mathbf{R}$, the evolution operator may be decomposed as in equations (10.13) and (10.14) into the form $U(\mathbf{R},t) = Z(\mathbf{R},t)\exp\{\mathrm{i}M(\mathbf{R})t\}$. This gives the instantaneous cyclic initial states $\phi_\alpha(\mathbf{R},0)$ and non-adiabatic Berry phases $\gamma_\alpha^N(\mathbf{R})$. Further, writing $\psi_\alpha(\mathbf{R},t) = Z(\mathbf{R},t)\phi_\alpha(\mathbf{R},0)$ gives a single-valued vector.

Now allow $\mathbf{R}$ to vary adiabatically with period $\tilde{t}_A = N\tilde{t}_N$. We can then state the generalised adiabatic ansatz: the initial state $\phi(0) = \phi_\alpha(\mathbf{R}(0),0)$ evolves into

$$\phi(t) = \exp\{\mathrm{i}\chi_\alpha(t)\}\psi_\alpha(\mathbf{R}(t),t). \tag{10.17}$$

As $\mathbf{R}(\tilde{t}_A) = \mathbf{R}(0)$ and $\psi_\alpha(\mathbf{R},\tilde{t}_A) = \psi_\alpha(\mathbf{R},0)$, the overall phase is just χ_α. To find the Berry phase we need merely note that equation (3.8) is applicable as $\psi_\alpha(\mathbf{R}(t),t)$ is a single-valued vector. Thus

$$\begin{aligned}\gamma_\alpha &= \mathrm{i}\int_0^{\tilde{t}_A} \langle\psi_\alpha(\mathbf{R}(t),t) \mid \dot{\psi}_\alpha(\mathbf{R}(t),t)\rangle \,\mathrm{d}t,\\ &= \Gamma_\alpha^N + \Gamma_\alpha^A,\end{aligned} \tag{10.18}$$

where

$$\Gamma_\alpha^N = \mathrm{i}\int_0^{\tilde{t}_A} \langle\phi_\alpha(\mathbf{R}(t),0) \mid Z^*(\mathbf{R}(t),t)\frac{\partial Z}{\partial t}(\mathbf{R}(t),t) \mid \phi_\alpha(\mathbf{R}(t),0)\rangle \,\mathrm{d}t, \tag{10.19}$$

$$\begin{aligned}\Gamma_\alpha^A = \mathrm{i}\int_0^{\tilde{t}_A} &\langle\phi_\alpha(\mathbf{R}(t),0) \mid Z(\mathbf{R}(t),t)\nabla_{\mathbf{R}}Z(\mathbf{R}(t),t) \mid \phi_\alpha(\mathbf{R}(t),0)\rangle \cdot \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\,\mathrm{d}t\\ &+ \mathrm{i}\int_0^{\tilde{t}_A} \langle\phi_\alpha(\mathbf{R}(t),0) \mid \nabla_{\mathbf{R}}\phi_\alpha(\mathbf{R}(t),0)\rangle \cdot \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\,\mathrm{d}t.\end{aligned} \tag{10.20}$$

To see why this is the correct splitting we need merely note that the derivative $\dot{\psi}_\alpha(\mathbf{R}(t),t)$ in equation (3.8) contains two parts. The first is the partial derivative with respect to time and is purely non-adiabatic (does not depend on the variation

of the parameters). The second part, which involves the partial derivative with respect to the parameters, is purely adiabatic.

Now we can break the integration from $t = 0$ to $t = \tilde{t}_A$ in equation (10.19) into the sum of integrations from $t = (n-1)\tilde{t}_N$ to $t = n\tilde{t}_N$ for $n = 1(1)N$. Further, as N is large and $\mathbf{R}$ is slowly varying, we can ignore the variation of $\mathbf{R}$ in each of these integrations. This allows us to replace $\mathbf{R}(t)$ by its value at the end of the integration range, namely $\mathbf{R}(n\tilde{t}_N)$. But then

$$\Gamma_N = \sum_{n=1}^{\infty} \gamma_\alpha^N(\mathbf{R}(n\tilde{t}_N)), \tag{10.21}$$

where each $\gamma_\alpha^N(\mathbf{R})$ is a normal non-adiabatic Berry phase. Hence in general we can decompose the Berry phase into the sum of non-adiabatic phases and a phase due to the adiabatic variation of some parameter $\mathbf{R}$ upon which the Hamiltonian H depends. Note that Simon *et al.* [1988] discuss a polarisation experiment where the parametric dependence of the non-adiabatic Berry phase is measured directly.

10.2 Breuer, Dietz and Holthaus' result

In the previous section we solved the problem of combining adiabatic and non-adiabatic time dependences by transforming the non-adiabatic problem into an equivalent time-independent form. The adiabatic variation could then be incorporated using the normal adiabatic theorem. Specifically, we started with the semi-classical Jaynes-Cummings model with adiabatically varying laser phase. Using the reduced density operator, the evolution for this system could be retrieved from the corresponding quantum model. Now, in the absence of any adiabatic parameter variation, the quantum model is a normal time-independent system. Hence the normal adiabatic theorem can be used once the parameters are allowed to vary.

We have already used a similar approach in chapter 6. There we started with a $\tilde{t}$-periodic Hamiltonian H on the Hilbert space $\mathcal{H}$. By using the Floquet Hamiltonian $K = H - \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$, the problem was converted into an effectively time-independent one on the Hilbert space $\mathcal{K} = \mathcal{T} \otimes \mathcal{H}$. In terms of the discussion of

the last paragraph, the expansion of the Hilbert space from $\mathcal{H}$ to $\mathcal{K}$ is equivalent to including photon degrees of freedom in the transition from the semi-classical to the quantum Jaynes-Cummings model. Thus we should be able to formalise the arguments of the previous section. We follow the work of Breuer and Holthaus [1989] and Breuer *et al.* [1990].

Now, as the elements of the Hilbert space $\mathcal{K}$ can be regarded as time-periodic vectors in the Hilbert space $\mathcal{H}$, a time parameter is needed in the description of the eigenvectors of the Floquet Hamiltonian. However, this is not the dynamical time in $\mathcal{K}$. To distinguish the two variables, we will label the eigenvectors with t and parameterise the time evolution with τ.

Our aim is to find the evolution of an initial state in $\mathcal{H}$ under the action of a given Hamiltonian $H(\mathbf{R})$ which contains two types of time variation. First, if $\mathbf{R}$ is held fixed, H is non-adiabatically periodic with period $\tilde{t}_N$. Second, the parameter $\mathbf{R}$ is adiabatically varied around a closed path with period $\tilde{t}_A$. In order that the Hamiltonian be $\tilde{t}_A$-periodic, we require that $\tilde{t}_A = N\tilde{t}_N$ for some (large) integer N. To solve this problem, we first solve the equivalent purely adiabatic problem in $\mathcal{K}$.

Let the parameterised Floquet Hamiltonian $K(\mathbf{R}) = H(\mathbf{R}) - \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$ have eigenvectors $\mid \epsilon_{\alpha n}(\mathbf{R})\rangle$ in $\mathcal{K}$:

$$K(\mathbf{R}) \mid \epsilon_{\alpha n}(\mathbf{R})\rangle = \epsilon_{\alpha n}(\mathbf{R}) \mid \epsilon_{\alpha n}(\mathbf{R})\rangle. \tag{10.22}$$

For convenience, we write the time evolution parameter as τ instead of t. This saves confusion when we interpret the $\mid \epsilon_{\alpha n}(\mathbf{R})\rangle$ as single-valued vectors in $\mathcal{H}$.

Now allow $\mathbf{R}$ to adiabatically vary about a closed path with period $\tilde{t}_A$. As $K(\mathbf{R}(\tau))$ is then a normal adiabatic Hamiltonian in $\mathcal{K}$, we can use the normal adiabatic theorem. Thus the time-dependent Schrödinger equation

$$\mathrm{i}\partial_\tau \Phi(\tau) = K(\mathbf{R}(\tau))\Phi(\tau) \tag{10.23}$$

has solutions of the form

$$\Phi(\tau) = \mathrm{e}^{\mathrm{i}\chi(\tau)} \mid \epsilon_{\alpha n}(\mathbf{R}(\tau))\rangle \tag{10.24}$$

for some phase $\chi(\tau)$. As $\mathbf{R}(\tilde{t}_A) = \mathbf{R}(0)$, the cyclic initial states are just the instantaneous eigenvectors $\mid \epsilon_{\alpha n}(\mathbf{R}(0))\rangle$ and the overall phases are just the $\chi(\tau)$. Further, by the analysis of section 3.1, the overall phase $\chi(\tilde{t}_A)$ is the sum of a Berry phase and a dynamical phase

$$\gamma^A_{\alpha n} = \mathrm{i}\int_0^{\tilde{t}_A} \langle\langle \epsilon_{\alpha n}(\mathbf{R}(\tau)) \mid \tfrac{\mathrm{d}}{\mathrm{d}\tau} \mid \epsilon_{\alpha n}(\mathbf{R}(\tau))\rangle\rangle \, \mathrm{d}\tau, \tag{10.25}$$

$$\delta^A_{\alpha n} = -\int_0^{\tilde{t}_A} \epsilon_{\alpha n}(\mathbf{R}(\tau)) \, \mathrm{d}\tau. \tag{10.26}$$

Note that the inner product on $\mathcal{K}$ is just

$$\langle\langle \cdot \mid \cdot \rangle\rangle = \frac{1}{\tilde{t}_N}\int_0^{\tilde{t}_N} \langle \cdot \mid \cdot \rangle \, \mathrm{d}t. \tag{10.27}$$

To relate this to the original Hamiltonian H, we interpret the $\mid \epsilon_{\alpha n}(\mathbf{R})\rangle$ as single-valued vectors $u_{\alpha n}(\mathbf{R}, t)$ in $\mathcal{H}$. Note that the parameter t, which will act as the evolution parameter in $\mathcal{H}$, is not the same as the evolution parameter τ in $\mathcal{K}$. Consider the vector

$$\phi(t) = \Phi(\tau, t) \mid_{\tau=t} \tag{10.28}$$

in $\mathcal{H}$. Then using the chain rule, we have

$$\begin{aligned} \mathrm{i}\partial_t \phi(t) &= \mathrm{i}\partial_\tau \Phi(\tau, t) \mid_{\tau=t} + \mathrm{i}\partial_t \Phi(\tau, t) \mid_{\tau=t} \\ &= K\Phi(\tau, t) \mid_{\tau=t} + \mathrm{i}\partial_t \Phi(\tau, t) \mid_{\tau=t} \\ &= H\Phi(\tau, t) \mid_{\tau=t} \\ &= H\phi(t). \end{aligned} \tag{10.29}$$

Hence the initial state $\phi(0)$ evolves into $\phi(t)$. Further, from equation (10.24) we can see that $\phi(0)$ is a cyclic initial state of H with overall phase $\chi(\tilde{t}_A)$.

In section 6.1, we saw that the eigenvectors of the Floquet Hamiltonian (taken at time $t = 0$) were precisely the cyclic initial states in the purely non-adiabatic case. Hence, in agreement with the previous section, in the mixed case

the cyclic initial states are just the instantaneous non-adiabatic cyclic initial states of $H(\mathbf{R}(0))$.

Using equations (10.25) and (10.26), Breuer *et al.* then state that the system has the Berry phase

$$\gamma^A_{\alpha n} = \mathrm{i}\int_0^{\tilde{t}_A} \langle\!\langle \epsilon_{\alpha n}(\mathbf{R}(\tau)) \mid \tfrac{\mathrm{d}}{\mathrm{d}\tau} \mid \epsilon_{\alpha n}(\mathbf{R}(\tau))\rangle\!\rangle \,\mathrm{d}\tau. \tag{10.30}$$

However, this does not agree with equation (10.18) above as it does not contain the non-adiabatic contributions. The reason for this discrepancy is that equation (10.26) for the dynamical phase assumes that the relevant energies are given by the $\epsilon_{\alpha n}(\mathbf{R})$ (the quasi-energies). While this is true for the quantum model, it is not the case for the semi-classical problem. In fact as shown in section 6.1, the quasi-energy gives the non-adiabatic overall phase, and so contains the non-adiabatic Berry phase as well as the dynamical phase. To be explicit, we break the integration in equation (10.26) into the sum of N pieces as in equation (10.21). For each piece, the variation of $\epsilon_{\alpha n}(\mathbf{R})$ due to $\mathbf{R}$ can be ignored giving

$$\begin{aligned}\delta^A_{\alpha n} &= \sum_{n=1}^{N} \epsilon_{\alpha n}(\mathbf{R}(n\tilde{t}_N))\tilde{t}_N \\ &= \sum_{n=1}^{N} (\gamma^N_{\alpha n} + \delta^N_{\alpha n}).\end{aligned} \tag{10.31}$$

Hence the Berry phase is the sum of adiabatic and non-adiabatic parts as in equation (10.18).

Breuer *et al.* [1990] note that this method is not appropriate for many systems with infinite-dimensional Hilbert spaces. This is because for the adiabatic theorem to hold in $\mathcal{K}$, the quasi-energies must be separated by gaps. However, for many systems the quasi-energy spectrum is dense on the real line and so the adiabatic theorem is not applicable. This subtlety does not arise in the example to be treated in the next section, as there the Hilbert space $\mathcal{H}$ is finite-dimensional.

10.3 An example

I now apply the theory developed above to a model two-level atom. Consider a two-level atom in a resonant laser, where the atomic transition is between an s state and a p_{-1} state split from the other p states by, say, a magnetic field. Now the electron-photon interaction has the electric dipole form $\mathbf{e}\cdot\mathbf{r}$, where $\mathbf{e}$ is the laser polarisation [Knight and Milonni 1980]. Let the laser have elliptical polarisation

$$\mathbf{e} = \sqrt{\tfrac{1}{2}}(1 - \mathrm{i}\cos\theta, \mathrm{i}\sin\theta, 0). \tag{10.32}$$

Later I will allow θ to vary adiabatically. We adopt the convention that at $\theta = -\pi/2$ the laser is left circularly polarised, while at $\theta = \pi/2$ it is right circularly polarised.

Using the fact that $p_{-1} \sim |\, x\rangle - \mathrm{i}\,|\, y\rangle$, we find that

$$\begin{aligned}\langle p_{-1} \mid H \mid s\rangle &= \langle p_{-1} \mid \mathbf{e}\cdot\mathbf{r} \mid s\rangle \mathrm{e}^{-\mathrm{i}\omega t} + \langle p_{-1} \mid \mathbf{e}^*\cdot\mathbf{r} \mid s\rangle \mathrm{e}^{\mathrm{i}\omega t} \\ &= \left(1 - \mathrm{i}\mathrm{e}^{-\mathrm{i}\theta}\right)\mathrm{e}^{-\mathrm{i}\omega t} + \left(1 + \mathrm{i}\mathrm{e}^{-\mathrm{i}\theta}\right)\mathrm{e}^{\mathrm{i}\omega t}.\end{aligned} \tag{10.33}$$

Thus, writing $\lambda = 1 + \mathrm{i}\exp\{\mathrm{i}\theta\}$ and $\mu = 1 - \mathrm{i}\exp\{\mathrm{i}\theta\}$, the semi-classical Hamiltonian is given by

$$H = \begin{bmatrix} \frac{\omega}{2} & k\left(\overline{\lambda}\mathrm{e}^{-\mathrm{i}\omega t} + \overline{\mu}\mathrm{e}^{\mathrm{i}\omega t}\right) \\ k\left(\lambda\mathrm{e}^{\mathrm{i}\omega t} + \mu\mathrm{e}^{-\mathrm{i}\omega t}\right) & -\frac{\omega}{2} \end{bmatrix}. \tag{10.34}$$

We can identify the rotating wave coupling constant λ and non-rotating wave coupling constant μ. Note that at $\theta = \pi/2$, the rotating wave coupling vanishes. This is a direct consequence of the selection rules for the $s \rightarrow p_{-1}$ transition.

It is important to note that this Hamiltonian is quite a crude approximation to the real state of affairs. There are several reasons for this. First, we make the electric dipole approximation. These terms, while small, are likely to be of at least the same order of magnitude as the non-rotating wave terms. Further, and more importantly, the other states in the p triplet will couple significantly even in the presence of a strong magnetic field. This will have important qualitative effects

on the dynamics of the problem. Nevertheless, the Hamiltonian (10.34) serves as a very useful model Hamiltonian for testing the calculational procedure derived in section 10.1, as well as providing a qualitative insight into the physical problem.

Before evaluating the adiabatic Berry phases for the problem, we calculate the non-adiabatic Berry phases that occur when θ is kept constant. To do this we use the formalism of section 6.1. As the problem cannot be solved exactly, we treat the rotating wave part of the interaction exactly and the counter-rotating part perturbatively. In fact, as the rotating wave coupling vanishes for some values of θ, we must use degenerate perturbation theory [Lindgren and Morrison 1985, pp184-208]. Putting $\mu = 0$, we find that the Floquet Hamiltonian has eigenvectors

$$| \epsilon^R_{\alpha n}\rangle = \sqrt{\tfrac{1}{2}} \mid -, n\rangle \pm \sqrt{\tfrac{1}{2}} \frac{\overline{\lambda}}{|\lambda|} \mid +, n-1\rangle, \tag{10.35}$$

with eigenvalues

$$\epsilon^R_{\alpha n} = (n - \tfrac{1}{2})\omega \pm k|\lambda|. \tag{10.36}$$

Note that at $\lambda = 0$, the quasi-energy states $| \epsilon_{\alpha n}\rangle$ are indeterminate. This is a consequence of the fact that H is degenerate at $\lambda = 0$ and will be dealt with later.

Reinstating μ, the first order quasi-energy states and quasi-energies can be found by degenerate perturbation theory. After considerable labour we find that

$$\epsilon_{\alpha n} = (n - \tfrac{1}{2})\omega \pm \sqrt{a^2 + b^2}, \tag{10.37}$$

$$\begin{aligned}
\frac{1}{N} \mid \epsilon_{\alpha n}\rangle = {} & \alpha_\pm \mid -, n\rangle + \frac{\overline{\lambda}}{|\lambda|}\beta_\pm \mid +, n-1\rangle \\
& + \frac{k\lambda\overline{\mu}}{4|\lambda|}\left(\alpha_\pm k|\lambda|\zeta - \beta_\pm(\omega^{-1} - \omega\zeta)\right) \mid -, n+2\rangle \\
& + \frac{k\overline{\mu}}{4}\left(-\beta_\pm k|\lambda|\zeta - \alpha_\pm(\omega^{-1} + \omega\zeta)\right) \mid +, n+1\rangle \\
& + \frac{k\overline{\lambda}\mu}{4|\lambda|}\left(-\alpha_\pm k|\lambda|\zeta + \beta_\pm(\omega^{-1} + \omega\zeta)\right) \mid -, n-2\rangle \\
& + \frac{k\mu\overline{\lambda}^2}{4|\lambda|^2}\left(\beta_\pm k|\lambda|\zeta + \alpha_\pm(\omega^{-1} - \omega\zeta)\right) \mid +, n-3\rangle,
\end{aligned} \tag{10.38}$$

where

$$N = \left(1 + \frac{k^2|\mu|^2}{8\omega^2}\left(1 + \frac{1 + k^2|\lambda|^2/\omega^2}{(1 - k^2|\lambda|^2/\omega^2)^2}\right)\right)^{-1/2}, \tag{10.39}$$

$$\alpha_+ = \beta_- = \frac{\left(\sqrt{a^2 + b^2} + a\right)^{1/2} + b\left(\sqrt{a^2 + b^2} + a\right)^{-1/2}}{2(a^2 + b^2)^{1/4}}, \tag{10.40}$$

$$\beta_+ = -\alpha_- = \frac{\left(\sqrt{a^2 + b^2} + a\right)^{1/2} - b\left(\sqrt{a^2 + b^2} + a\right)^{-1/2}}{2(a^2 + b^2)^{-1/4}}, \tag{10.41}$$

$$a = k|\lambda|\left(1 - \frac{k^2|\mu|^2}{4\omega^2}\left(1 - k^2|\lambda|^2\omega^2\right)^{-1}\right), \tag{10.42}$$

$$b = -\frac{k^2|\mu|^2}{4\omega}\left(1 + \left(1 - k^2|\lambda|^2/\omega^2\right)\right)^{-1}, \tag{10.43}$$

$$\zeta = (\omega^2 - k^2|\lambda|^2)^{-1}. \tag{10.44}$$

Thus, after applying equation (6.4), we find that the cyclic initial states $\phi_\pm(0)$ are given by

$$\phi_\pm(0) = N\begin{bmatrix} l_\pm \\ m_\pm \end{bmatrix}, \tag{10.45}$$

where

$$m_+ = \frac{\lambda}{|\lambda|}(1 + \mathrm{i}k^2\cos\theta\zeta)\alpha_+ - \frac{\mathrm{i}k\cos\theta\lambda}{\omega|\lambda|^2}\beta_+, \tag{10.46}$$

$$l_+ = (1 + \mathrm{i}k^2\cos\theta\zeta)\beta_+ - \frac{\mathrm{i}k\cos\theta}{\omega|\lambda|}\alpha_+, \tag{10.47}$$

$$m_- = (1 + \mathrm{i}k^2\cos\theta\zeta)\alpha_- - \frac{\mathrm{i}k\cos\theta}{\omega|\lambda|}\beta_-, \tag{10.48}$$

$$l_- = \frac{\overline{\lambda}}{|\lambda|}(1 + \mathrm{i}k^2\cos\theta\zeta)\beta_- - \frac{\mathrm{i}k\cos\theta\overline{\lambda}}{\omega|\lambda|^2}\alpha_-. \tag{10.49}$$

Note that the singularity in $\lambda/|\lambda|$ is not a problem. This is because at $\theta = \pi/2$, which is where $\lambda/|\lambda|$ is indeterminate, α_+ and β_- vanish so that the offending terms do not contribute to m_+ or l_-. Further, the terms in $\lambda\cos\theta/|\lambda|^2$ are well-behaved in the limit $\theta \to \pi/2$.

We can also calculate the Berry phases from equation (6.17), giving

$$\gamma_\pm^N = 2\pi N^2\left(\beta_\pm^2 - X\right), \tag{10.50}$$

where X is a constant of order $k^2|\mu|^2/\omega^2$. This result is interesting in its own right, especially if we consider the special cases of $\theta = \pm\pi/2$, corresponding to right and left circularly polarised light respectively. For a left circularly polarised laser, the non-rotating wave coupling constant μ is zero and so we see only the rotating wave interaction. This is not particularly useful as the rotating wave contribution is dominant anyway. Of more interest is the case of a right circularly polarised laser, for which the rotating wave coupling λ is zero and we see the non-rotating wave coupling, which is usually hidden.

In theory, the non-rotating wave coupling could be observed by measuring the splitting of the Mollow triplet [Knight and Milonni 1980]. In section 9.1, this quantity was shown to be proportional to the difference in overall phases of the two electronic cyclic initial states. However, as mentioned at the start of this section, there are many complicating factors such as magnetic dipole terms and admixing of the other states in the p triplet.

As discussed in section 9.3, few authors have considered the effect of the non-rotating wave coupling. For example, Phoenix [1989] shows that the counter-rotating term can induce a small phase-dependent term into the expression for the atomic inversion, but also notes that one would expect the two-level approximation to fail before the rotating wave one. Thus arguments about the measurability of non-rotating wave terms in the two-level atomic model are in some sense academic. Note, however, that the inclusion of these terms is of crucial importance in the calculation of the adiabatic Berry phases that arise when the phase parameter is varied, as we will now see.

We now allow θ to vary from zero to π (or equivalently from $\pi/2$ to $5\pi/2$). The resulting adiabatic Berry phase is given by equation (10.20):

$$\Gamma_{\pm}^{A} = \mathrm{i}\int_{0}^{2\pi} \langle \phi_{\pm} \mid \tfrac{\mathrm{d}}{\mathrm{d}\theta} \mid \phi_{\pm} \rangle \, \mathrm{d}\theta. \tag{10.51}$$

To evaluate this, we take only the leading terms in the expansion of $\phi_{\pm}(0)$. For $\phi_{-}(0)$,

$$l_{-} = \frac{\overline{\lambda}}{|\lambda|}\beta_{-} \qquad \text{and} \qquad m_{-} = \alpha_{-}. \tag{10.52}$$

Now, as $\overline{\lambda}/|\lambda|$ has unit magnitude, it is a phase, $\exp\{-\mathrm{i}f(\theta)\}$. At $\theta = \pi/2$, $\overline{\lambda}/|\lambda|$ jumps from $-\mathrm{i}$ to i and so f jumps from $\pi/2$ to $-\pi/2$. Thus $f(\theta+2\pi) = f(\theta)+\pi$. Also, using the fact that α_- and β_- are both real, we find that equation (10.52) gives

$$\Gamma_-^A = \int_{\pi/2}^{5\pi/2} \dot{f}\beta_-^2 \, \mathrm{d}\theta. \tag{10.53}$$

Thus all we need to do is calculate β_-.

To leading order we have

$$a = k|\lambda| \qquad \text{and} \qquad b = \frac{-k^2|\mu|^2}{4\omega}. \tag{10.54}$$

Now $|a|$ is much larger than $|b|$ for all θ except for a small interval around $\theta = \pi/2$. Further, this small interval does not contribute to the adiabatic Berry phase in lowest order and can be ignored. This allows us to take $\beta_- = 1/\sqrt{2}$ from equation (10.40). Hence the adiabatic Berry phase is given by $\Gamma_-^A = \pi/2$. We can similarly show that $\Gamma_+ = -\pi/2$. Thus we see a complex phase change. This contrasts, for example, with the case of a time-reversal even adiabatic Hamiltonian. As elegantly shown by Kivelson and Rokhsar [1988], these systems can only have Berry phases of zero or π. More examples of the effects of time-reversal odd coupling are given in appendix C.

This behaviour is due to the fact that our chosen polarisation path takes the system through a point ($\lambda = 0$) where the rotating wave eigenvectors of the Floquet Hamiltonian are degenerate. To see why this is so, consider the problem in the rotating wave approximation with arbitrary rotating wave coupling constant. Then for fixed λ, the Floquet Hamiltonian has eigenvectors

$$|\,\epsilon_{\alpha n}^R\rangle = \sqrt{\tfrac{1}{2}}\,|-,n\rangle \pm \sqrt{\tfrac{1}{2}}\frac{\overline{\lambda}}{|\lambda|}\,|+,n-1\rangle \tag{10.55}$$

as before. Hence, writing $\overline{\lambda}/|\lambda| = \exp\{-\mathrm{i}f\}$, the adiabatic Berry phase is given by $f(\tilde{t}_A)/2$ (assuming that $f(0) = 0$ for simplicity). Now, for the eigenvectors to be single-valued, we must have $f(\tilde{t}_A) = 2m\pi$. This gives the Berry phase as zero

or π. Of course this is not due to time-reversal invariance, the system containing time-odd terms due to breaking of the chiral symmetry of the p states.

To get a complex phase, the path must be taken through the degeneracy at $\lambda = 0$ as was done above. At first sight this causes problems, as the degeneracy at $\lambda = 0$ means that the adiabatic theorem should not hold. However the counter-rotating term splits the two states, restoring its validity. Travelling through the degeneracy also means that $\overline{\lambda}/|\lambda|$ need no longer be single-valued. This is because, near the degeneracy, the magnitude of the coefficients of the basis elements $|-, n\rangle$ and $|+, n-1\rangle$ are no longer constant as in equation (10.55), so that the coefficient of $\overline{\lambda}/|\lambda|$ could vanish at the degeneracy. If this is the case, any jump in $\overline{\lambda}/|\lambda$ at the degeneracy will not spoil the single-valuedness of the eigenvectors. This is exactly what happens in our example. At $\theta = \pi/2$ we find that f jumps by π, generating the Berry phase $\pi/2$. Hence the non-rotating wave terms are of crucial importance in enabling complex Berry phases to exist.

Chapter Eleven

Extensions

In section 3.1, I defined the cyclic initial states of a $\tilde{t}$-periodic Hamiltonian H as those states $\phi(0)$ that return to themselves up to a phase at time $\tilde{t}$. This phase is called the overall phase and has two parts. The first is the natural generalisation of the dynamical phase that is present in the evolution of the stationary states of a time-independent system. The second part is of geometrical origin and is called the Berry phase.

These definitions can be extended in many different ways, some of which have already been discussed. To see where generalisations are possible, we need to analyse the restrictions that the standard definitions impose. The first is that the Hamiltonian is taken to be periodic. This assumption provides a natural final time (the period of the Hamiltonian) and enables us to use the formalisms of sections 5.1 and 6.1. However, as we have already seen in section 9.2, this restriction can be relaxed. For example, Zak [1989] discusses adiabatic Hamiltonians that are only periodic up to a gauge transformation.

We also assume that the Hamiltonian is self-adjoint, so that the evolution is unitary. This restriction was relaxed in section 9.3, where I discussed the inclusion of spontaneous emission in the Jaynes-Cummings model. The evolution can even be punctuated by measurements [Benedict and Fehér 1989]. Generalisation to non-potential Lie-isotopic systems is also possible [Mignani 1988].

Further, we have defined the Berry phase in the quantum context. However, it turns out that there is a classical analogue, utilising the action-angle variables, called the Hannay angle [Hannay 1985, Berry 1985]. A simple physical system exhibiting these angles is the Foucault pendulum [Aitchison 1990]. Note that

the classical system can even be non-integrable, as long as it has some symmetry [Montgomery 1988]. It can be shown that the geometric formalism of section 7.1 has a counterpart in the classical case [Golin *et al.* 1989, Weinstein 1990].

In the next two sections, I briefly discuss some other important generalisations. The standard definitions require the existence of a cyclic initial state. This is relaxed in two different ways in section 11.1. First I consider cyclic initial spaces. The elements of these spaces do not necessarily come back to themselves up to a phase, but they must at least come back to some other member of the set. The reducing subspaces discussed in section 8.1 are obvious examples. This generalisation was first reported by Wilczek and Zee [1984] for adiabatic systems, and Anandan [1988] for the non-adiabatic case.

Next, I generalise the definition of the phase difference between two states in such a way that it can be used for vectors that are not on the same ray in Hilbert space. In this way Berry phases can be defined for arbitrary initial states. In fact, we will see that there are two non-equivalent definitions. One is physically motivated [Samuel and Bhandari 1988]. The other defines the phase difference as an observable (that is, as a self-adjoint operator).

Of course the most general states in quantum mechanics are not the vectors of the Hilbert space, but the density operators. These operators include statistical mixtures and are the basis of the algebraic formulation of quantum theory [Emch 1984, pp361-382]. We find that the definition of Berry phases can be extended to cover all initial density operators, not just those corresponding to pure states. This generalisation is due to Uhlmann [1989] and Dabrowski and Grosse [1990]. Finally, the standard definition of the Berry phase assumes that the system is described by a Hamiltonian. This restriction is dropped in section 11.4, following the work of Jordan [1988a].

11.1 The initial states

The standard definition of the Berry phase requires the existence of a cyclic initial wavefunction. As outlined above, there are three ways to relax this restriction: one can consider cyclic initial spaces, non-cyclic evolutions or initial density operators. These generalisations are the subject of this section.

First we discuss cyclic initial spaces. Let $\mathcal{M}$ be a subspace of the Hilbert space $\mathcal{H}$ such that $U(\tilde{t})\mathcal{M} = \mathcal{M}$. Then any initial state in $\mathcal{M}$ returns to $\mathcal{M}$. Mathematically, $\mathcal{M}$ is said to reduce the monodromy operator. A simple example is the one-dimensional subspace generated by some cyclic initial state $\phi(0)$. For this case, the restriction of the monodromy operator $U(\tilde{t})$ to $\mathcal{M}$ is just the overall phase $\exp\{\mathrm{i}\chi\}$. With this in mind, for a general reducing subspace $\mathcal{M}$ we define the "overall phase" to be the restriction of the monodromy operator to $\mathcal{M}$. This definition was first proposed by Wilczek and Zee [1984] for the adiabatic case, and was generalised to the non-adiabatic case by Anandan [1988].

Another example is an eigenspace of an operator that commutes with the Hamiltonian $H(t)$ at all times. Reducing spaces of this kind were used in section 8.1 when I discussed the existence of cyclic initial states. These reducing spaces were shown to have a basis of cyclic initial states. In fact this property holds for any finite-dimensional reducing subspace. Thus, analysing cyclic initial spaces just corresponds to allowing linear combinations of some set of cyclic states to be used as initial states.

This fact can be used to display explicitly the geometric part of the monodromy operator $U(t)$ [Anandan 1988]. The reducing subspace $\mathcal{M}$ has a basis $\{\phi_\alpha(0)\}$ of cyclic initial states. Let $\{\psi_\alpha(t)\}$ be a corresponding set of single-valued vectors. Then the evolution operator can be written

$$U(t) = \mathcal{T}\exp\{\mathrm{i}\int_0^t (A - K)\,\mathrm{d}t'\}, \tag{11.1}$$

where $\langle\psi_\alpha(t) \mid A \mid \psi_\beta(t)\rangle = \mathrm{i}\langle\psi_\alpha \mid \dot{\psi}_\beta\rangle$ and K is simply related to the instantaneous expectation values of the Hamiltonian. As K gives the dynamical part of the evolution operator, A represents the geometrical part.

This identification is stronger when A and H commute. Then we have

$$U(t) = \mathcal{T}\exp\{-\mathrm{i}\int_0^t H\,\mathrm{d}t\}\exp\{\mathrm{i}\int_0^t A\,\mathrm{d}t\}, \tag{11.2}$$

and the dynamical and geometric parts are separated. This situation occurs in the adiabatic case considered by Wilczek and Zee [1984]. They analysed an adiabatic Hamiltonian $H(t)$ with a k-fold degenerate eigenspace $\mathcal{M}(t)$. Then, by the adiabatic theorem, an initial state in $\mathcal{M}(0)$ returns to that eigenspace. Further, all states in this space have the same dynamical phase. This means that H is a multiple of unity in $\mathcal{M}(t)$ and so must commute with A.

Note that this problem can also be treated geometrically as in section 7.1. The only difference is that the base space of the fibre bundle must be taken to be the Grassmann manifold of k-dimensional subspaces of $\mathcal{H}$, instead of the projective Hilbert space of one-dimensional subspaces [Giler *et al.* 1989].

We can also define Berry phase for arbitrary evolutions. There are two non-equivalent ways of doing this. One is physically motivated, while the other displays the overall phase as an observable. First consider the physically motivated definition. Let ϕ_1 and ϕ_2 be two non-orthogonal vectors. We define their phase difference χ to be the phase of their inner product [Jordan 1988b]. That is,

$$r\mathrm{e}^{\mathrm{i}\chi} = \langle\phi_1 \mid \phi_2\rangle. \tag{11.3}$$

This is called the Pancharatnam phase. Note that if the two vectors are on the same ray in Hilbert space, then the Pancharatnam phase is just the normal phase difference. This definition has already been used in section 9.2, where I discussed Berry phases for the Rabi oscillation.

This definition is motivated by the interference of light beams. Consider the interference intensity

$$\begin{aligned}\|\phi_1 + \phi_2\|^2 &= 2 + r\mathrm{e}^{\mathrm{i}\chi} + r\mathrm{e}^{-\mathrm{i}\chi} \\ &= 2(1 + \cos\chi)\,.\end{aligned} \tag{11.4}$$

Then if $\chi = 0$, that is if ϕ_1 and ϕ_2 are "in phase", the intensity is maximal. However, if $\chi = \pi$ so that the two vectors are "out of phase", the resultant intensity is minimal. Hence the definition (11.3) is physically reasonable.

In applications to Berry phase, we take ϕ_1 to be the initial state $\phi(0)$ and ϕ_2 to be the final state $\phi(\tilde{t})$. The Berry phase is then defined to be the geometrical part of the Pancharatnam phase. As with the normal Berry phase, this phase can be directly calculated from the system's path in projective Hilbert space [Samuel and Bhandari 1988]. This definition has been applied to, for example, neutron beam experiments [Weinfurter and Badurek 1990] and quantum optics [Moore 1990c].

Unfortunately, the Pancharatnam phase does not give the overall phase the status of an observable, that is it is not a self-adjoint operator. This is because the process of taking the phase of the inner product $\langle\phi(0) \mid \phi(\tilde{t})\rangle$ is essentially non-linear. However, it is possible to define an overall phase operator. Given the monodromy operator $U(\tilde{t})$, there exists a unique self-adjoint operator X, with spectrum in $[0, 2\pi)$, such that $U(\tilde{t}) = \exp\{\mathrm{i}X\}$ (see section A.1). For instance, if the Hamiltonian is $\tilde{t}$-periodic, then $X = M\tilde{t}$, where M is defined in section 5.1.

Now the cyclic initial states $\phi_\alpha(0)$ are the eigenvectors of X, the overall phases being the corresponding eigenvalues. Thus the operator X is a natural overall phase operator. The overall phase of an arbitrary initial state is just the expectation value of X in that state. However, while this definition is natural mathematically, it does not have the physical motivation of Pancharatnam's definition. This is because $\langle\exp\{\mathrm{i}X\}\rangle \neq \exp\{\mathrm{i}\langle X\rangle\}$, so that $\|\phi(0) + \exp\{\mathrm{i}X\}\phi(0)\| \neq 2(1 + \cos\chi)$.

Note that non-cyclic evolutions can also be treated geometrically [Anandan and Aharonov 1990]. For a given evolution $\phi(t)$, define the number

$$s = 2\int \Delta E(t)\,\mathrm{d}t, \tag{11.5}$$

where the energy uncertainty $\Delta E(t)$ is given by

$$\Delta E^2 = \langle\phi \mid H^2 \mid \phi\rangle - \langle\phi \mid H \mid \phi\rangle^2. \tag{11.6}$$

Anandan and Aharonov prove that, like the Berry phase, s only depends on the path C followed by the system in projective Hilbert space. Thus it is indeed a geometric quantity (the distance along C as measured by the Fubini-Study metric). This metric has also been studied in the quantum mechanical context by von Baltz [1990].

Now let $\pi(\psi_1)$ and $\pi(\psi_2)$ be the projections of the states ψ_1 and ψ_2 onto the projective Hilbert space. Then Anandan and Aharonov prove that

$$|\langle\psi_1 \mid \psi_2\rangle|^2 = \cos^2 \tfrac{\theta}{2}, \tag{11.7}$$

where θ is the distance along the shortest geodesic joining $\pi(\psi_1)$ and $\pi(\psi_2)$. Hence, as mentioned in section 4.2, transition probabilities can be described geometrically.

The last extension I will consider in this section is that to initial density operators. We could use the operator definition above, defining the overall phase of the density operator $\rho(0)$ to be $\mathrm{Tr}(\rho(0)X)$. However there is also a geometric definition, due to Uhlmann [1989] and Dabrowski and Grosse [1990]. They use the projection map $\pi' : A \mapsto AA^*$ of the space of Hilbert-Schmidt operators into the space of density operators. This may be compared to the method of section 7.1, where the standard projection of the Hilbert space into the projective Hilbert space was used.

11.2 The Berry phase without dynamics

Up until now, we have been concerned with the evolution of states (pure or mixed) under the action of a Hamiltonian (self-adjoint or non-self-adjoint). In this section I define Berry phases without the use of a Hamiltonian, that is without dynamics. This definition, due to Jordan [1988a], uses a complete set of commuting self-adjoint operators to generate the "evolution" of an initial eigenvector. One can tie this definition back to the usual one by suitable definition of the system Hamiltonian.

Consider a complete set of commuting self-adjoint operators $A_1, A_2, \ldots$ with simultaneous eigenbasis $\mid m\rangle$:

$$A_j \mid m\rangle = a_m^{(j)} \mid m\rangle. \tag{11.8}$$

Note that, as the set $\{A_j\}$ is complete, only one label is needed for the eigenbasis. The "dynamics" is provided by a unitary operator $U(q)$, where $q \in [0, Q]$, satisfying the following three conditions:

$$U(0) = 1, \tag{11.9}$$

$$\forall j, \quad [U(Q), A_j] = 0, \tag{11.10}$$

$$\forall m, \quad \langle m \mid U^*(q)G(q)U(q) \mid m\rangle = 0, \tag{11.11}$$

where $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}U(q) = G(q)U(q)$. Note that condition (11.8) is very similar to the condition used in section 7.1.

We now define the evolution of the operators A_j. Put

$$A_j(q) = U(q)A_jU^*(q). \tag{11.12}$$

Then equations (11.9) and (11.10) imply that

$$A_j(Q) = A_j = A_j(0). \tag{11.13}$$

Further, as $U(Q)$ commutes with all of the members of the complete set $\{A_j\}$, it must be a function of them, namely

$$U(Q) = \mathrm{e}^{-\mathrm{i}\alpha(A_1, A_2, \ldots)}. \tag{11.14}$$

In particular,

$$U(Q) \mid m\rangle = \mathrm{e}^{-\mathrm{i}\alpha(a_m^{(1)},a_m^{(2)},\ldots)} \mid m\rangle. \tag{11.15}$$

This leads to the following definition: the Berry phases of the states $\mid m\rangle$ are given by

$$\gamma_m = -\alpha(a_m^{(1)}, a_m^{(2)}, \ldots). \tag{11.16}$$

For example, consider the Berry phases generated from the two-dimensional Lorentz group [Jordan 1988a]. This group is generated by the operators K_1, K_2 and J_3 with the commutation relations

$$[K_1, K_2] = -\mathrm{i}J_3, \qquad [K_2, J_3] = \mathrm{i}K_1 \qquad \text{and} \qquad [J_3, K_1] = \mathrm{i}K_2. \tag{11.17}$$

Now, since the eigenvectors of J_3 form a non-degenerate set,

$$J_3 \mid m\rangle = m \mid m\rangle, \tag{11.18}$$

J_3 is a complete set of commuting operators. Let $\mathbf{k}(q)$ be a real three-vector with

$$-k_1(q)^2 - k_2(q)^2 + k_3(q)^2 = 1 \tag{11.19}$$

and $\mathbf{k}(0) = (0, 0, 1) = \mathbf{k}(Q)$. Then we define the operator $A(q)$ of equation (11.9) by

$$A(q) = k_1(q)K_1 + k_2(q)K_2 + k_3(q)J_3. \tag{11.20}$$

Note that there is only one A as there is only one commuting operator. Further, we have that $A(0) = J_3 = A(Q)$.

Now define the operator $G(q)$ by

$$\begin{aligned} G(q)\,\mathrm{d}q = {} & (k_2\,\mathrm{d}k_3 - k_3\,\mathrm{d}k_2)K_1 + (k_3\,\mathrm{d}k_1 - k_1\,\mathrm{d}k_3)K_2 \\ & - (k_1\,\mathrm{d}k_2 - k_2\,\mathrm{d}k_1)J_3. \end{aligned} \tag{11.21}$$

We find that $A(q) = U(q)A(0)U^*(q)$, where $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}U(q) = G(q)U(q)$ and $U(0) = 1$. Further, we have that

$$\langle m \mid U^*(q)G(q)U(q) \mid m\rangle = 0. \tag{11.22}$$

Now, as $U(Q)$ and J_3 commute, $U(Q)$ must be a function of J_3. Further, $U(Q)$ is a product of unitary operators generated by K_1, K_2 and J_3. Thus

$$U(Q) = \mathrm{e}^{-\mathrm{i}\phi J_3}, \tag{11.23}$$

and so the state $\mid m\rangle$ has Berry phase $\gamma_m = -m\phi$.

We now turn back to the general development. The vectors $\mid \zeta_m(q)\rangle = U(q) \mid m\rangle$ fulfil the role of the vectors in equation (7.1). It is then natural to ask if there are any vectors that play the part of the single-valued vectors. It is easy to see that we can take the vector $\mid \psi_m(q)\rangle = \exp\{-\mathrm{i}\theta_m(q)\} \mid \zeta_m(q)\rangle$, where $\theta_m(Q) = \gamma_m(Q)$. Further,

$$\begin{aligned}
&\tfrac{\mathrm{d}}{\mathrm{d}q} \mid \psi_m(q)\rangle = -\mathrm{i}\dot{\theta}_m \mid \psi_m(q)\rangle - \mathrm{i}G(q)U(q)\mathrm{e}^{-\mathrm{i}\theta_m(q)} \mid m\rangle \\
\Rightarrow \quad &\dot{\theta}_m = \mathrm{i}\langle\psi_m(q) \mid \tfrac{\mathrm{d}}{\mathrm{d}q} \mid \psi_m(q)\rangle \\
\Rightarrow \quad &\gamma_m = \mathrm{i}\int_0^Q \langle\psi_m(q) \mid \tfrac{\mathrm{d}}{\mathrm{d}q} \mid \psi_m(q)\rangle\,\mathrm{d}q,
\end{aligned} \tag{11.24}$$

where I have used equation (11.8). This is just the normal result for the Berry phase in terms of a single-valued vector.

Jordan's definition can be linked to dynamics by the appropriate choice of Hamiltonian. Let

$$H(t) = gG(q) + \sum_m E_m(t)U(q) \mid m\rangle\langle m \mid U^*(q), \tag{11.25}$$

where g and $E_m(t)$ are parameters and $t = q/g$. Define the final time by $T = Q/g$. Note that H is not necessarily T-periodic, but this is not important. I will now show that this Hamiltonian has cyclic initial states $\mid m\rangle$ and single-valued vectors $\mid \psi_m(q)\rangle$. This motivates the definition (11.13).

By direct substitution, we find that the vector $|\,\phi_m(0)\rangle = |\,m\rangle$ evolves into

$$|\,\phi_m(t)\rangle = \mathrm{e}^{-\mathrm{i}\omega(t)}U(q)\,|\,m\rangle, \tag{11.26}$$

where $\omega_m(t) = \int_0^t E_m(t')\,\mathrm{d}t'$. Further,

$$\begin{aligned} |\,\phi_m(T)\rangle &= \mathrm{e}^{-\mathrm{i}\omega_m(T)}U(Q)\,|\,m\rangle \\ &= \mathrm{e}^{-\mathrm{i}\omega_m(T)}\mathrm{e}^{\mathrm{i}\gamma_m}\,|\,\phi_m(0)\rangle. \end{aligned} \tag{11.27}$$

Hence $|\,m\rangle$ is indeed a cyclic initial state. Further, as $|\,\psi_m(q)\rangle$ is equal to the evolving state up to a phase, it is a suitable single-valued vector. Thus the generalised definition (11.13) of the Berry phase reduces to the standard one in the case of Hamiltonian evolution.

Chapter Twelve

Conclusion

We have developed a new approach for the calculation of Berry phases for periodic, but not necessarily adiabatic, Hamiltonians. This utilises an evolution operator decomposition scheme made possible by the periodicity of the Hamiltonian (section 5.1). This periodicity can be further exploited to express the Berry phases for the system directly in terms of the Fourier expansion of the Hamiltonian (section 6.1).

This formalism is important from a theoretical viewpoint for several reasons. First, it allows the relationship between the Berry phase and the time dependence of the Hamiltonian to be clearly delineated (section 5.2). Further, the operator decomposition scheme greatly aids the resolution of such questions as the existence of cyclic initial states (section 8.3).

On the practical level, our formalism is particularly useful for the analysis of two-level atomic problems. For example, it allows one to interpret the frequency of the Rabi oscillation and the splitting of the Mollow triplet (section 9.1). Further, the Rabi oscillation can itself be investigated (section 9.2). Finally, it leads to a modified adiabatic ansatz for systems with superimposed adiabatic and non-adiabatic evolutions (section 10.1).

To highlight the relationship between our results and other approaches, the work of other authors in this field has been surveyed (sections 7.1 and 7.2). We find that, calculationally at least, all of these methods merely provide us with single-valued vectors (section 3.1).

Our work can be extended in many ways. For example, it would be useful to examine other systems using our formalism. There is also room for further investigation of the use of Berry phase to interpret known phenomena, such as the

Mollow splitting.

On the theoretical side, more work is needed in the characterisation of which systems have cyclic initial states and which do not. For example, it would be valuable to formulate necessary and sufficient conditions for the existence of a complete set of cyclic initial states in terms of the spectral decomposition of the Hamiltonian.

Appendix A

Mathematical preliminaries

In this appendix I briefly discuss some of the mathematical results used in the rest of the thesis. More detail can be found, for example, in Choquet-Bruhat *et al.* [1982] and Conway [1985].

In section A.1 I discuss functional analysis. After some preliminary definitions, the spectral theorem is stated. This is then used to prove that any unitary operator is the exponential of an anti-self-adjoint one. This result is crucial in the proof of the existence of the evolution operator decomposition of section 5.1.

In section A.2, attention is turned to the theory of connections on principal fibre bundles. The notion of a connection is shown to lead to the definition of holonomy. Further, I show that holonomy can be used to give a geometric interpretation of the Berry phase.

A.1 Functional analysis

The operator decomposition scheme of section 5.1 requires a little operator theory. In this section I state the theorems that we need. These can be derived from the spectral theorem, which gives the spectral decomposition of an arbitrary normal operator. First a few definitions. More detail can be found in Conway [1985] and Weidmann [1980].

Let $\mathcal{H}$ be a Hilbert space and $\mathcal{D}(A)$ be a subspace of $\mathcal{H}$. Then a *linear operator* A is a linear function

$$A : \mathcal{D}(A) \to \mathcal{H}. \tag{A.1}$$

$\mathcal{D}(A)$ is called the *domain* of A and is often required to be dense. A is called *bounded* if $||A\phi|| \leq C||\phi||$ for some constant C and all $\phi \in \mathcal{D}(A)$. Otherwise it is *unbounded.*

A good example of an unbounded operator is the position operator q. Note that all unitary operators are bounded as they preserve norms. Bounded operators are much easier to deal with than unbounded ones. Unfortunately, many operators of importance in quantum mechanics (such as the harmonic oscillator Hamiltonian) are not bounded.

Next we discuss the spectrum. This includes the eigenvalues of the operator and a continuous part. We need the following definition. Let A be a linear operator. Then A is *boundedly invertible* if there is a bounded operator B such that $AB = 1$ and $BA \subseteq 1$. Here $X \subseteq Y$ iff $\mathcal{D}(X) \subseteq \mathcal{D}(Y)$ and the two operators agree on $\mathcal{D}(X)$. This leads to the following definition. If A is an operator, then the *spectrum* of A is the set

$$\sigma(A) = \{\lambda \in \mathbb{C} \mid \lambda - A \text{ is not boundedly invertible}\}. \tag{A.2}$$

We also need the concepts of self-adjointness and unitarity. Let A be an operator. Then A is *self-adjoint* if $A^* = A$ and *unitary* if $AA^* = A^*A = 1$. Here A^* is the adjoint of A. As mentioned above, unitarity implies boundedness. Note

that the spectrum of a self-adjoint operator is a subset of $\mathbb{R}$, and the elements of the spectrum of a unitary operator are all complex numbers with unit norm. Further, an operator is normal if $A^*A = AA^*$. Both self-adjoint and unitary operators are normal.

The final definition we need before stating the spectral theorem is that of a *spectral measure*. Let X be a set, Ω be a σ-algebra of subsets of X and $\mathcal{H}$ be a Hilbert space. Further, let $\mathcal{B}(\mathcal{H})$ be the algebra of bounded operators on $\mathcal{H}$. Then a *spectral measure* for $(X, \Omega, \mathcal{H})$ is a function $E : \Omega \to \mathcal{B}(\mathcal{H})$ satisfying the following conditions:

(i) For each $\Delta \in \Omega$, $E(\Delta)$ is a projection,
(ii) $E(\emptyset) = 0$ and $E(X) = 1$,
(iii) $E(\Delta_1) \cap E(\Delta_2) = E(\Delta_1)E(\Delta_2)$ for all $\Delta_1, \Delta_2 \in \Omega$,
(iv) If $\{\Delta_n\}_{n=1}^{\infty}$ are pairwise disjoint sets in Ω, then $E(\cup_{n=1}^{\infty}\Delta_n) = \sum_{n=1}^{\infty} E(\Delta_n)$.

The following result lets us integrate with respect to a spectral measure. The proof can be found in Conway [1985, p328].

Theorem A.1 *Let E be a spectral measure for $(X, \Omega, \mathcal{H})$ and $f : X \to \mathbb{C}$ be an Ω-measurable function. For $\phi, \psi \in \mathcal{H}$, let $E_{\phi\psi}$ be the complex-valued measure defined by $E_{\phi\psi}(\Delta) = \langle E(\Delta)\phi \mid \psi \rangle$ for each $\Delta \in \Omega$. Then there is a unique operator N such that*

$$\mathcal{D}(N) = \{\phi \in \mathcal{H} \mid \int |f^2| \, \mathrm{d}E_{\phi\phi} < \infty\}, \tag{A.3}$$

$$\langle N\phi \mid \psi \rangle = \int f \, \mathrm{d}E_{\phi,\psi}. \tag{A.4}$$

We write $N = \int f \, \mathrm{d}E$.

We are now in a position to state the spectral theorem. The proof can be found in Conway [1985, p330].

Theorem A.2 *Let N be a normal operator on the Hilbert space $\mathcal{H}$. Then there is a unique spectral measure E defined on the Borel subsets of $\mathbb{C}$ such that:*

(i) $N = \int z \, \mathrm{d}E$,

(ii) $E(\Delta) = 0$ *if* $\Delta \cap \sigma(N) = \emptyset$,

(iii) *If* U *is an open subset of* $\mathbb{C}$ *and* $U \cap \sigma(N) \neq \emptyset$, *then* $E(U) \neq 0$,

(iv) *If* $A \in \mathcal{B}(\mathcal{H})$ *such that* $AN \subseteq NA$ *and* $AN^* \subseteq N^*A$, *then* $A(\int f \, \mathrm{d}E) \subseteq (\int f \, \mathrm{d}E)A$ *for every Borel function* f *on* $\mathbb{C}$.

If N is bounded, the spectral theorem can be simplified. We have [Conway 1985, p269]

Theorem A.3 *Let* N *be a bounded normal operator on the Hilbert space* $\mathcal{H}$. *Then there is a unique spectral measure* E *on the Borel subsets of* $\sigma(N)$ *such that:*

(i) $N = \int z \, \mathrm{d}E$,

(ii) *If* G *is a nonempty relatively open subset of* $\sigma(N)$ *then* $E(G) \neq 0$,

(iii) *If* $A \in \mathcal{B}(\mathcal{H})$, *then* $AN = NA$ *and* $AN^* = N^*A$ *iff* $AE(\Delta) = E(\Delta)A$ *for every* Δ.

Note that these results allow us to define functions of operators. For if $N = \int z \, \mathrm{d}E$ and f is a measurable complex-valued function, we can put

$$f(N) = \int f(z) \, \mathrm{d}E. \tag{A.5}$$

The spectral theorem allows us to prove that for every unitary operator U, there is a unique self-adjoint operator X, with spectrum in $[0, 2\pi)$, such that $U = \exp\{\mathrm{i}X\}$. This result is used in the operator decomposition of section 5.1. I follow Jordan [1969].

As U is bounded, there is a unique spectral measure E on the Borel subsets of $\sigma(U)$ such that

$$U = \int z \, \mathrm{d}E. \tag{A.6}$$

Now as mentioned earlier this section, the spectrum of a unitary operator is contained in the set of complex numbers with unit norm. Hence we can write equation

(A.6) in the form

$$U = \int \mathrm{e}^{\mathrm{i}x}\,\mathrm{d}E, \tag{A.7}$$

where x is real. Further, if we restrict x to the interval $[0, 2\pi)$, then this representation is unique.

Now consider the bounded operator

$$X = \int x\,\mathrm{d}E. \tag{A.8}$$

Then X is a bounded normal operator. But we can also see that its spectrum lies in the real axis. Hence it is self-adjoint. Finally, by the definition of a function of an operator, we have that $U = \exp\{iX\}$. This completes the proof.

A related result is Stone's theorem [Conway 1985, p337]. Let $U(t)$ be a strongly continuous time-dependent unitary operator $U(t)$ satisfying $U(s+t) = U(s)U(t)$. Then Stone's theorem states that $U(t)$ may be written in the form $U(t) = \exp\{\mathrm{i}At\}$ for some constant self-adjoint operator A. A is bounded iff $\lim_{t\to 0} \|U(t) - 1\| = 0$.

A.2 Fibre bundles

In section 7.1, the Berry phase was shown to be the holonomy of the natural connection of the Hopf bundle. I now explain this terminology. The treatment given here is based on that of Choquet-Bruhat *et al.*[1982, p125]. After giving the general definitions, the particular case of the Hopf bundle is explained.

Let E and B be differentiable manifolds and $\pi : E \to B$ be a continuous surjection. Then (E, B, π) is called a *bundle*. We restrict our attention to those bundles for which $\pi^{-1}(x)$ is homeomorphic to some manifold F for all x. F is then called the *typical fibre*. We call B the *base space* and E the *total space*.

Intuitively, this means that E should be related to $B \times F$ in some way. Pinning down this relationship leads to the definition of a fibre bundle. Now it is to restrictive to require that E be equal to $B \times F$. Thus we will only take the fibre bundle to be a product locally. That is, we require the existence of an open cover $\{U_j\}$ of B such that $\pi^{-1}(U_j)$ is homeomorphic to $U_j \times F$.

For this definiton to be useful, we need the patches U_j to "match". This leads to the existence of a set of conditions on the homeomorphisms $\phi_j : \pi^{-1}(U_j) \to U_j \times F$ [Choquet-Bruhat *et al.* 1982, p126]. We note that these are stated in terms of a Lie group G of homeomorphisms of the typical fibre F onto itself. Hence the fibre bundle is written (E, B, π, G). Note that any two points in a given fibre are related by a unique element of the structure group G. This fact will be very useful in the definition of holonomy.

A trivial example of a fibre bundle is given by taking $E = B \times G$. Here the typical fibre F and Lie group G are identical, and G acts on the fibre by right translation. A fibre bundle whose typical fibre and structure group coincide is called a *principal fibre bundle*.

Let C_B be a path in the base space of a given principal fibre bundle. Then there are many paths C_E in the total space that project onto C_B. These are called *lifts*. Our aim is to pick out a distinguished one of these.

To do this we need to be able to compare points on different fibres. This

leads to the definition of a connection. It turns out to be convenient to define connections in terms of the tangent vectors to paths in E. Specifically, let $T_p(E)$ be the tangent space at $p \in E$. This has a natural subspace $V_p(E) = T_p(G_x)$ of vectors tangent to the fibre in which p lies [Choquet-Bruhat, 1982, p.359]. Now for each $p \in E$, let $H_p(E)$ be a complementary subspace to $V_p(E)$. That is

$$T_p(E) = H_p(E) \oplus V_p(E). \tag{A.9}$$

This assignment is called a *connection.*

Note that $H_p(E)$ is not unique. For example, let $T_p(E) = \mathbb{R}^2$ and $V_p(E)$ be the linear span of $(0,1)$. Then the only restriction on the basis vector $\mathbf{u}$ of $H_p(E)$ is that it cannot be collinear with (0,1). For this case, an obvious choice of connection is the orthogonal subspace to $V_p(E)$. That is, we can take $H_p(E)$ to be the linear span of $(1,0)$. We can define a *natural connection* in this way whenever the tangent space has a natural inner product. This will be very important when I discuss the Hopf bundle.

The reason the connection is useful is that it generates a distinguished lift for a given curve in the base space of the bundle. This lift is defined by requiring that the tangent vector of the path in E be horizontal. For this reason it is often called the *horizontal lift.*

We are now in a position to define holonomy. This concept is used in section 7.1 to describe the geometrical nature of the Berry phase. Consider a closed curve C_B in the base space of a given principal fibre bundle. Then the corresponding horizontal lift C_E in the total space is not necessarily closed. In fact the initial point p_i and final point p_f of C_E need only be in the same fibre. This means that they are connected by an element of the structure group G. In other words,

$$p_f = p_i g \tag{A.10}$$

for some $g \in G$. This group element is called the *holonomy.* Note that the holonomy depends upon the choice of connection used to define the horizontal lift.

For applications to Berry phase, the total space is taken to be the space $\mathcal{N}$ of normalised states and the base space is taken to be the projective Hilbert space $\mathcal{H}$. Hence π is just the natural projection,

$$\pi : \mathcal{N} \to \mathcal{P} : \phi \mapsto |\, \phi\rangle\langle\phi \,|\,. \tag{A.11}$$

This gives a principal fibre bundle with structure group $U(1)$, called the Hopf bundle [Chern 1977].

Now the tangent space at a given point of $\mathcal{N}$ is just the parent Hilbert space $\mathcal{H}$. As this has an inner product, there is a natural connection, defined by taking the orthogonal complement of $V_\phi(\mathcal{N})$ at each $\phi \in \mathcal{N}$. Further, as the structure group is $U(1)$, the holonomy of this connection will just be multiplication by a phase. I will now show that this holonomy is the Berry phase. I follow Bohm *et al.*[1990].

First we must identify the vertical subspace $V_\phi(\mathcal{N})$. In fact, as we can regard ϕ as a vector in either $\mathcal{N}$ or $\mathcal{H}$, the vertical subspace is just the linear span of ϕ. Hence the natural connection is defined by requiring the horizontal vectors in $T_\phi(\mathcal{N})$ to be orthogonal to ϕ.

Now, if $\phi(t)$ is a curve in $\mathcal{N}$, then its tangent vector in $\mathcal{H}$ is just $\dot{\phi}(t)$. Thus the lift $\phi(t)$ of a curve in $\mathcal{P}$ is horizontal iff

$$\langle\phi \mid \dot{\phi}\rangle = 0. \tag{A.12}$$

The holonomy is then given by

$$\mathrm{e}^{\mathrm{i}\theta} = \langle\phi(0) \mid \phi(\tilde{t})\rangle, \tag{A.13}$$

where ϕ satisfies equation (A.12) and the closed path in $\mathcal{P}$ takes time $\tilde{t}$. But from equations (7.1)-(7.3), this means that the holonomy of the natural connection is just the Berry phase.

Appendix B

Coherent states

In this appendix I discuss coherent states. These are used in section 7.2 (Lie algebraic approaches to the calculation of Berry phases) and section 8.2 (the existence of cyclic initial states for the forced harmonic oscillator). They are also necessary to describe the photon statistics of a laser operating well above threshold, which is used in the Jaynes-Cummings model.

Coherent states were first used by Glauber [1963] in quantum optics, his definition being based on the work of Schrödinger [1926]. Besides these applications, coherent states have found their way into many areas of physics, for example the path integral formulation of quantum mechanics [Klauder 1960].

The rest of this appendix is organised as follows. In section B.1 I give the properties of the standard coherent states that are used in the rest of this work. The account is by no means complete, with topics such as the minimal uncertainty of the coherent states [Nussenzveig 1973, p47] and their relationship to entire analytic functions [Bargmann 1961] being left out. In section B.2 the statistics of lasers operating well above threshold is discussed. Finally, in section B.3 I discuss generalised coherent states. Explicit forms of the $SU(2)$ and $SU(1,1)$ coherent states, which are used in section 7.2, are also given.

B.1 Standard coherent states

We start with the boson creation and annihilation operators a^* and a satisfying the canonical commutation relation

$$[a, a^*] = 1. \tag{B.1}$$

These have a concrete representation in terms of the position q and momentum p; we can take

$$a = \sqrt{\tfrac{1}{2}}(q + ip) \tag{B.2}$$

and its conjugate. The Hilbert space then has a basis $\{\mid n\rangle\}$ of eigenvectors of the number operator: $a^*a \mid n\rangle = n \mid n\rangle$. The creation and annihilation operators act as follows

$$a \mid n\rangle = \sqrt{n} \mid n-1\rangle, \tag{B.3}$$

$$a^* \mid n\rangle = \sqrt{n+1} \mid n+1\rangle. \tag{B.4}$$

Thus, in terms of the vacuum $\mid 0\rangle$, the number states can be written as

$$\mid n\rangle = \frac{a^{*n}}{\sqrt{n!}} \mid 0\rangle. \tag{B.5}$$

The coherent states $\mid z\rangle$ are defined to be the eigenvectors of a. As the number states are complete, we can write $\mid z\rangle = \sum_{n=0}^{\infty} \langle n \mid z\rangle \mid n\rangle$. Then

$$\begin{aligned} \langle n \mid z\rangle &= \frac{1}{\sqrt{n!}} \langle 0 \mid a^n \mid z\rangle \\ &= \frac{z^n}{\sqrt{n!}} \langle 0 \mid z\rangle. \end{aligned} \tag{B.6}$$

Now, as z is normalised,

$$\begin{aligned} 1 &= \sum_{n=0}^{\infty} |\langle 0 \mid z\rangle|^2 \frac{|z|^{2n}}{n!} \\ &= \mathrm{e}^{|z|^2} |\langle 0 \mid z\rangle|^2. \end{aligned} \tag{B.7}$$

Thus we may take $\langle 0 \mid z\rangle = \exp\{-|z|^2/2\}$ so that

$$\mid z\rangle = \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} \mid n\rangle. \tag{B.8}$$

Note that z can be any complex number so that a has an uncountable set of eigenvectors. This is in contrast to the case of an arbitrary self-adjoint operator (such as a^*a). As their eigenspaces are mutually orthogonal, they can only have a countable number of eigenvalues (as every separable Hilbert space has a countable basis).

We also note that the creation operator a^* does not have any eigenvalues. To see why this is so, let $\mid \alpha\rangle = \sum_{n=0}^{\infty} \alpha_n \mid n\rangle$ be a non-zero eigenvector of a^* with eigenvalue α. Using equation (B.4), we can directly compare the expansions of $a^* \mid \alpha\rangle$ and $\alpha \mid \alpha\rangle$ in the number state basis, giving

$$a^* \mid \alpha\rangle = \sum_{n=1}^{\infty} c_{n-1}\sqrt{n} \mid n\rangle, \tag{B.9}$$

$$\alpha \mid \alpha\rangle = \sum_{n=0}^{\infty} c_n \alpha \mid n\rangle. \tag{B.10}$$

Note that the sum in (B.9) is from $n = 1$ while that in equation (B.10) is from $n = 0$. Equating coefficients we have that c_0 and $c_n = (\sqrt{n}/\alpha)c_{n-1}$. But this implies that all of the c_n are zero which contradicts our initial assumption.

The coherent states (B.8) can be expressed in another simple form. In fact, this is the form generated by the Lie algebraic method of section B.3. We need the following lemma [Nussenzveig 1973, p45] which I state without proof.

Lemma B.1 *Let A and B be two operators which commute with their commutator $[A, B]$. Then* $\exp\{A\}\exp\{B\} = \exp\{[A, B]/2\}\exp\{A + B\}$.

Let $A = za^*$ and $B = -\overline{z}a$. Then $[A, B] = |z|^2[a, a^*] = |z|^2$ which commutes with both A and B. Now consider the vector $\mid z\rangle' = \exp\{za^* - \overline{z}a\} \mid 0\rangle$. Applying lemma B.1, we have

$$\mid z\rangle' = \mathrm{e}^{-|z|^2/2}\mathrm{e}^{za^*}\mathrm{e}^{-\overline{z}a} \mid 0\rangle. \tag{B.11}$$

Now, as $a \mid 0\rangle = 0$, we have that $\exp\{-\overline{z}a\} \mid 0\rangle = \mid 0\rangle$. Thus

$$\begin{aligned} \mid z\rangle' &= \mathrm{e}^{-|z|^2/2}\mathrm{e}^{za^*} \mid 0\rangle \\ &= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2/2} \frac{z^n a^{*n}}{n!} \mid 0\rangle \\ &= \sum_{n=0}^{\infty} \mathrm{e}^{-|z|^2} \frac{z^n}{\sqrt{n!}} \mid n\rangle. \end{aligned} \tag{B.12}$$

Hence we can write the coherent state $\mid z\rangle$ in the form

$$\mid z\rangle = \mathrm{e}^{za^* - \overline{z}a} \mid 0\rangle. \tag{B.13}$$

Next we find the statistics of the coherent state, that is the probability of finding the system in the state $\mid n\rangle$. We have that $P_n = \exp\{-|z|^2\}|z|^{2n}/n!$, the Poisson distribution [Laha and Rohatgi 1979, p31]. We can simply calculate the mean and variance of this distribution:

$$\langle n\rangle = \langle z \mid a^*a \mid z\rangle = |z|^2, \tag{B.14}$$

$$\begin{aligned} \langle n^2\rangle - \langle n\rangle^2 &= \langle z \mid a^*aa^*a \mid z\rangle - |z|^4 \\ &= |z|^2\langle z \mid aa^* \mid z\rangle - |z|^4 \\ &= |z|^2\langle z \mid a^*a + 1 \mid z\rangle - |z|^4 = |z|^2. \end{aligned} \tag{B.15}$$

Note that as n tends to infinity, the distribution becomes sharply peaked as the ratio of the standard deviation to the mean tends to zero. This result is of crucial importance in the derivation of the semi-classical limit of the Jaynes-Cummings model presented in section 2.2.

The number states possess a spectral resolution of unity: $\sum_{n=0}^{\infty} \mid n\rangle\langle n \mid = 1$. It turns out that the coherent states have a similar property. We need the following lemma:

Lemma B.2 $\int_0^{\infty} r^{2n+1}\exp\{-r^2\}\,\mathrm{d}r = n!/2$.

Proof: We proceed by induction. For $n = 0$ we have

$$\begin{aligned} \int_0^{\infty} r\mathrm{e}^{-r^2}\,\mathrm{d}r &= -\tfrac{1}{2}[\mathrm{e}^{-r^2}]_0^{\infty} \\ &= \frac{0!}{2}. \end{aligned} \tag{B.16}$$

Assume that the lemma is true for $n = k$ so that $\int_0^\infty r^{2k+1}\exp\{-r^2\}\,\mathrm{d}r = k!/2$. Then, by induction,

$$\int_0^\infty r^{2(k+1)+1}\mathrm{e}^{-r^2}\,\mathrm{d}r = -\tfrac{1}{2}[r^{2(k+1)}\mathrm{e}^{-r^2}]_0^\infty + (k+1)\int_0^\infty r^{2k+1}\mathrm{e}^{-r^2}\,\mathrm{d}r$$
$$= \frac{(k+1)!}{2}, \qquad (B.17)$$

completing the proof. ∎

Now consider $\int \mid z\rangle\langle z \mid \mathrm{d}^2z/\pi$. We have

$$\tfrac{1}{\pi}\int \mid z\rangle\langle z \mid \mathrm{d}^2z = \tfrac{1}{2}\sum_{n,m=0}^{\infty}\frac{\mid m\rangle\langle n \mid}{\sqrt{m!}\sqrt{n!}}\int \overline{z}^m z^n \mathrm{e}^{-|z|^2}\,\mathrm{d}^2z$$
$$= \tfrac{1}{\pi}\sum_{n,m=0}^{\infty}\frac{\mid m\rangle\langle n \mid}{\sqrt{m!}\sqrt{n!}}\int_0^\infty r^{m+n+1}\mathrm{e}^{-r^2}\int_0^{2\pi}\mathrm{e}^{\mathrm{i}(n-m)\theta}\,\mathrm{d}\theta$$
$$= 2\sum_{n=0}^{\infty}\frac{\mid n\rangle\langle n \mid}{n!}\int_0^\infty r^{2n+1}\mathrm{e}^{-r^2}\,\mathrm{d}r$$
$$= \sum_{n=0}^{\infty}\mid n\rangle\langle n \mid = 1. \qquad (B.18)$$

This is the generalisation of the number state spectral resolution of unity.

Equation (B.18) implies that the coherent states are complete. However, there are an uncountable number of them and so they cannot be pairwise orthogonal. I will now show that in fact no two coherent states are orthogonal. Further, we will see that no two distinct coherent states are equal up to a phase. To do this we evaluate the inner product of two arbitrary coherent states $\mid z\rangle$ and $\mid z'\rangle$. We have

$$\langle z' \mid z\rangle = \mathrm{e}^{-|z'|^2/2}\mathrm{e}^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{\overline{z}'^n z^n}{n!}$$
$$= \exp\{-|z'|^2/2 + \overline{z}'z - |z|^2/2\}. \qquad (B.19)$$

This has square modulus

$$|\langle z' \mid z\rangle|^2 = \exp\{-|z'|^2 + \overline{z}'z + z'\overline{z} - |z|^2\}$$
$$= \mathrm{e}^{-|z'-z|^2}. \qquad (B.20)$$

As this is never zero or unity (for $z' \neq z$), no two distinct coherent states are orthogonal or collinear.

B.2 Laser statistics

In this section I show that a laser operating well above threshold has Poisson statistics. The treatment given here follows Stenholm [1973]. Imagine that the field is initially in the state ρ_f^0 and we inject excited two-level atoms into the cavity with rate r_1. Further, we assume that each atom contributes independently. Then we can evaluate the evolved joint density operator $\rho(t)$ using the Liouville equation $\mathrm{i}\dot{\rho} = [H, \rho]$, where H is simply the quantum Jaynes-Cummings Hamiltonian.

We are only interested in the field, so we trace out the atomic variables to give the reduced density operator. Actually, we are really only interested in the diagonal elements ρ_{nn} of the reduced density operator, as these are the probabilities of finding the system in a state with n photons.

As yet we have not taken account of losses in the system. To do this we introduce another set of atoms into the cavity, initially in the ground state. If they are injected at the rate r_2, then one can show that the diagonal matrix elements $\rho_{nn}(t)$ of the reduced density operator satisfy the coupled differential equations

$$\dot{\rho}_{nn} = -\frac{A(n+1)}{1+(n+1)B/A}\rho_{nn} + \frac{An}{1+nB/A}\rho_{n-1,n-1} - Cn\rho_{nn} + C(n+1)\rho_{n+1,n+1}. \qquad (B.21)$$

Here $A = r_1 2\lambda^2/\gamma^2$, $B = (4\lambda^2/\gamma^2)A$ and $C = r_2 2\lambda^2/\gamma_2^2$. Here λ is the atom-field coupling constant, γ^{-1} is the average lifetime of the excited atoms and γ_2^{-1} is that of the ground state atoms.

This relation can also be derived heuristically by identifying A as a linear amplification factor, B as a saturation factor and C as a loss factor [Loudon 1983, p272]. Although the transient time evolution of the ρ_{nn} is hard to find from equation (B.21), we may easily obtain the steady state solution by setting $\dot{\rho}_{nn} = 0$.

This leads to the recursion relation

$$\rho_{n+1,n+1} = \frac{A/C}{1+(n+1)B/A}\rho_{nn}, \tag{B.22}$$

which has the solution

$$\rho_{nn} = \rho_{00}(A/C)^n \prod_{k=1}^{n}(1+kB/A)^{-1}. \tag{B.23}$$

There are two special cases of particular interest. If A is much smaller than C, then intuitively the system's losses outweigh its gains, and we say that the laser is below threshold. The solution (B.23) is then approximately given by

$$\rho_{nn} = (1-A/C)(A/C)^n. \tag{B.24}$$

By introducing the temperature $\theta = -(k_B/\omega)A/C$ we can see that this is the black body distribution. On the other hand, if we take $A \gg C$, then the distribution (B.23) tends to the limit

$$\rho_{nn} = \frac{(A/B)^n}{n!}\mathrm{e}^{-(A/B)}. \tag{B.25}$$

This is just the Poisson distribution. Therefore a laser operating well above threshold may be represented by a coherent state.

B.3 Generalised coherent states

The definition of coherent states presented in section B.1 can be extended in many ways. In this section I will concentrate on the Lie algebraic definition of Perelomov [1972]. This gives us the $SU(2)$ and $SU(1,1)$ coherent states which are used in section 7.2. Other extensions, such as atomic coherent states [Arecchi *et al.* 1972], vector coherent states [Rowe *et al.* 1985] and coherent states over symplectic homogeneous spaces [De Bièvre 1989], will not be discussed.

The development of the generalised coherent states given here follows Perelomov [1986]. Consider a Lie group G with a unitary irreducible representation T on the Hilbert space $\mathcal{H}$. Fix a vector $\mid \psi_0\rangle$ in $\mathcal{H}$. This is called the fiduciary vector and in applications is often taken to be the vacuum $\mid 0\rangle$. We define the system of states $\{\mid \psi_g\rangle\}$ by $\mid \psi_g\rangle = T(g) \mid \psi_0\rangle$, where g runs over the Group G. We will define the coherent states in terms of this system.

The reason we cannot use the set $\{\mid \psi_g\rangle\}$ directly is that it contains many linearly dependent subsets. In fact, let H be the isotropy subgroup for $\mid \psi_0\rangle$, that is the maximal subgroup of elements h such that $T(h) \mid \psi_0\rangle = \exp\{\mathrm{i}\alpha(h)\} \mid \psi_0\rangle$. Then the two states $\mid \psi_{g'}\rangle$ and $\mid \psi_g\rangle$ are equal up to the phase $\alpha(h)$ iff $g' = gh$. Thus the states we need are the equivalence classes of the factor group $X = G/H$. To exhibit them explicitly, we choose a representative $g(x)$ of each equivalence class x in X. In other words, the coherent states are the set $\{\mid x\rangle \equiv \mid \psi_{g(x)}\rangle\}$. Note that G can be considered as a fibre bundle with base space $X = G/H$ and fibre H. The choice of the $g(x)$ is then just the choice of a cross-section. It can be shown that properties such as completeness then follow from the irreducibility of the representation T.

This definition can be used to regenerate the standard coherent states of section B.1. To do this we need the Heisenberg-Weyl algebra W_1. This is the real three-dimensional Lie algebra generated by the commutation relations

$$[e_1, e_2] = e_3, \qquad [e_1, e_3] = 0 \qquad \text{and} \qquad [e_2, e_3] = 0. \tag{B.26}$$

For example we may take $e_1 = \mathrm{i}p$, $e_2 = \mathrm{i}q$ and $e_3 = \mathrm{i}1$. Thus an arbitrary element

of W_1 may be written in the form

$$\begin{aligned} x &= x_1 e_1 + x_2 e_2 + s e_3 \\ &= \mathrm{i}s1 + (\alpha a^* - \overline{\alpha} a). \end{aligned} \tag{B.27}$$

To get the elements of the corresponding Lie group we exponentiate:

$$g = \mathrm{e}^x = \mathrm{e}^{\mathrm{i}s1} \mathrm{e}^{\alpha a^* - \overline{\alpha} a}. \tag{B.28}$$

It is easy to see that for all fiduciary states, the isotropy subgroup consists of those elements of the form $h = \exp\{\mathrm{i}s1\}$. To get the standard coherent states we choose $\mid \psi_0\rangle = \mid 0\rangle$ and take the equivalence class representatives with $s = 0$. Thus

$$\mid \alpha\rangle = \mathrm{e}^{\alpha a^* + \overline{\alpha} a} \mid 0\rangle, \tag{B.29}$$

in agreement with equation (B.13).

Two other cases will concern us here, namely the $SU(2)$ and $SU(1,1)$ coherent states. The Lie algebra of $SU(2)$ is generated by

$$[J_0, J_\pm] = \pm J_\pm, \qquad [J_-, J_+] = -2J_0. \tag{B.30}$$

We find that the coherent states are given by

$$\mid \xi\rangle = \mathrm{e}^{\xi J_+ - \overline{\xi} J_+} \mid \psi_0\rangle. \tag{B.31}$$

Finally, the Lie algebra of $SU(1,1)$ is generated by

$$[K_0, K_\pm] = \pm K_\pm, \qquad [K_-, K_+] = 2K_0. \tag{B.32}$$

A concrete realisation in terms of the creation and annihilation operators is

$$K_+ = \tfrac{1}{2}(a^*)^2, \qquad K_- = \tfrac{1}{2}a^2, \qquad K_0 = \tfrac{1}{4}(aa^* + a^*a). \tag{B.33}$$

Here the coherent states are given by

$$\mid \zeta\rangle = \mathrm{e}^{\zeta K_+ - \overline{\zeta} K_-} \mid \psi_0\rangle. \tag{B.34}$$

Appendix C
Time reversal

In this appendix I survey the effects that time-reversal odd coupling could have on ion-lattice interactions [Moore and Stedman 1990a]. This study was undertaken during the first six months of my doctoral research and, among other things, helps to explain the effect time-reversal has on the values the Berry phase may take.

At first sight, one might argue that all systems must be time-reversal invariant due to the CPT theorem [Sachs 1987, p36]. However this is not the case. This is because the theorem only holds for isolated systems. In focussing our attention on one part of the system (effectively treating the rest of it classically), we allow the presence of time-odd interactions. A good example is an atom in an external magnetic field. This may be compared to the presence of Hamiltonian time dependence. An isolated system must have a time-independent Hamiltonian. However, as discussed in section 2.2, time dependence can be induced by the coupling of the system to its surroundings.

Of particular interest here are ligand-field systems, in which we analyse the interactions of a given ion with the motion of its surrounding ligands. The usual model of the interaction treats the ligands merely as a quasi-static electron distribution [Abragam and Bleaney 1970]. Hence the interaction is taken to be time-reversal even. But this is not the only possible mechanism. For example, there will be an induced Zeeman term. This comes from the fact that the motion of the charged ligands induces a magnetic field. Hence it is time-reversal odd.

Time-odd coupling has largely been ignored in the literature. For example, Gill [1975] states "It is accepted that the effect on the paramagnetic ion of the electromagnetic fields which are associated with the vibrations of the lattice is

quite negligible". There are several reasons for this neglect. The first is that the principal mechanism for spin-lattice relaxation of paramagnetic ions in crystals is clearly the electrostatic one. This, along with the failure of the time-odd direct spin-spin mechanism prposed by Waller [1932], points to the dominance of time-even coupling. Another reason that time-odd interactions are largely ignored is the fact that back-of-the-envelope calculations indeed suggest that they are small.

However, there are serious objections to the out of hand dismissal of time-odd effects. For example, Fletcher [1981] establishes a direct connection between the induced Zeeman coupling and the Barnett effect of magnetisation by rotation. This effect has been observed in many systems [Bates 1961].

Further, back-of-the-envelope calculations of any mechanism can prove to be totally inadequate. For example, the static ligand field is known to be poorly predicted. In fact, for lanthanides the higher order parameters can be underestimated on a point charge model by up to two orders of magnitude. A similar "quantum enhancement" could be expected for the time-odd mechanism.

Finally, it is unlikely that the semi-classical Zeeman effect is the dominant interaction. Before rejecting the possible relevance of time-odd coupling, one might first be expected to formulate the theory of a Dirac electron in a molecule with internal motion (say in a rotating frame). In view of the plethora of relativistic terms which appear in the static solution of the Hamiltonian of a hydrogen atom, we may expect that such a calculation would throw up many dynamic terms of a time-odd character. Most of these would have no classical counterpart and some would be of at least comparable magnitude to the classical terms.

It is interesting to note the relationship between time-reversal odd coupling and rotational modes of the lattice. For example, consider momentum coupling in the D_4 Jahn-Teller system discussed in section 4.2. There the central ion coupled by a time-odd mechanism to the A_2 lattice mode. This is just the joint rotation of the ligands about the central ion. In fact, as we will now show, rotational modes always transform in a way which is inconsistent with time-even coupling.

The coupling must be odd at the $O(3)$ level, since the appropriate rotational

irrep 1^+ is never in the symmetric part of the square of any $O(3)$ irrep. This is preserved in branching through a subgroup chain, as the symmetric and antisymmetric parts of a Kronecker product do not mix under branching provided no multiplicities arise. Further, multiplicities arise only for point groups of relatively low symmetry, where any degeneracy may be assigned to partners within $1^{\pm}(O(3))$ for the purposes of a point group Kronecker product analysis. Finally, these multiplicities can always be removed by introducing an intermediate group. Thus rotational modes can only couple via a time-reversal odd mechanism.

We concede that the time-odd coupling is small. However, it may be possible to observe it in some systems. This is because there are often selection rules that lead to a total or partial cancellation of time-even couplings at lowest order in perturbation. Thus, while the time-reversal odd coupling is numerically smaller than the time-even, it can sometimes have an effect at a lower order of perturbation.

The rest of this appendix is organised as follows. In section C.1 the time-reversal selection rules are discussed following Stedman and Butler [1983]. In section C.2, these are used to find systems where time-odd effects could be seen. For instance, the sum rules for the reduction factors of the D_4 Jahn-Teller systems are broken by the presence of time-reversal odd coupling.

C.1 Selection rules

Consider a system with symmetry point group G. We are interested in the restriction time-reversal places upon the matrix elements of an irreducible tensor operator O^{μ}_{m}. As we will see, these restrictions often lead to the cancellation or near cancellation of time-reversal even couplings in first order perturbation theory. As these cancellations are circumvented by time-odd mechanisms, such systems could show time-reversal odd effects.

Let the Hilbert space of interest have basis $\{|\ \Lambda l\rangle\}$. We require the basis to be time-even in the sense that $\overline{|\ \Lambda l\rangle}$ should be expressible as a linear combination of the $|\ \Lambda l'\rangle$. Note that the overbar represents the time-reversed ket. For instance, if we take $G = O(3)$, then the basis $\{|\ \alpha j, m\rangle\}$ is time-even as $\overline{|\ \alpha j, m\rangle} = \epsilon(-1)^{j-m}|\ \alpha, j-m\rangle$. For general point groups, the requirement that the basis be time-even may necessitate taking Λ to be a reducible representation under G.

Now let τ_Λ be the phase of the basis under double time inversion. This is just $(-1)^n$ for an n-electron system. Further, let τ_O be the time-reversal signature of the operator of interest. Then, for the matrix elements

$$M_{ll'm} = \overline{\langle \Lambda l\ |} O^{\mu}_{m}\ |\ \Lambda l'\rangle \tag{C.1}$$

not to all vanish, we must have [Stedman and Butler 1983]

$$\mu_r \in [\Lambda \otimes \Lambda]_{\pm} \qquad \text{as} \quad \tau_\Lambda \tau_O = \pm 1. \tag{C.2}$$

Here r labels the possible repetitions of μ in the Kronecker product. In our applications we will enlarge the basis to the product $\{|\ \Lambda l\rangle\ |\ L\rangle\}$ of kets $|\ \Lambda l\rangle$ from the electronic space and kets $|\ L\rangle$ from the non-electronic space (photons or phonons or both) coupled by the interaction.

We shall also require an extension of this result. Consider the case where O is an effective operator derived from perturbation theory and bilinear in two

interactions A^α and B^β:

$$O = \sum_{\Omega\omega L} \Big(\sum_{L''} \frac{\langle L \mid A^\alpha \mid \Omega\omega \rangle \mid L'' \rangle \langle L'' \mid \langle \Omega\omega \mid B^\beta \mid L' \rangle}{E_\Lambda - E_\Omega + E_L - E_{L''}} + \sum_{L'''} \frac{\langle L \mid B^\beta \mid \Omega\omega \rangle \mid L''' \rangle \langle L''' \mid \langle \Omega\omega \mid A^\alpha \mid L' \rangle}{E_\Lambda - E_\Omega + E_L - E_{L'''}} \Big). \qquad (C.3)$$

Here $\{\Omega\omega\rangle\}$ is a basis for another (or possibly the same) electronic level, also assumed to be time-even. $\mid L\rangle$ symbolises the altered state of any non-electronic part of the system, for example photons or phonons. Note that we do not give O any suffices as the expansion (C.3) has not yet been written as a sum of irreducible tensor operators.

This type of operator occurs in processes in which the energy change in going from $\mid L\rangle$ to $\mid L'\rangle$ in the non-electronic system balances the energy change in the overall electronic transition. The labels L'' and L''' have been distinguished for the following reason. If A^α and B^β represent different processes, then the states $\mid L''\rangle$ and $\mid L'''\rangle$ will necessarily involve different quanta. Hence they will also have different energies. For brevity, I will refer to this as the case of *non-equivalent denominators*.

We find that the selection rule (C.2) is now only approximate. That is the requirement that

$$\mu_r \in [\Lambda \otimes \Lambda]_\pm \qquad \text{as} \quad \tau_A \tau_B \tau_\Lambda = \pm 1 \qquad (C.4)$$

only holds to the extent that the energy denominators of the two terms in equation (C.3) are equal.

In the next section, I will show that the conventional time-even mechanism for many physical processes is subject to a total or near cancellation through time-reversal considerations. In the latter case, a full cancellation is only avoided through the inequivalence of the energy denominators in equation (C.3). The time-even process is therefore intrinsically handicapped by the ratio of the difference of the denominators to their average. The time-odd coupling, although inherently much weaker, does not suffer this handicap and so could become significant.

C.2 Examples

In this section I will discuss three systems for which a time-reversal odd coupling could be observed in principle. More details can be found in Moore and Stedman [1990a].

C.2.1 Spin-lattice relaxation

First I consider the spin-lattice relaxation of Kramers systems. In EPR experiments on Kramers systems, the relaxation of interest occurs between two states in the set $\{|\ \Lambda l\rangle\}$ which correspond to some level. In the absence of any magnetic field, these two states will be degenerate. For simplicity we consider a doublet ground state $|\ a\rangle \sim |\ \frac{1}{2}, \frac{1}{2}\rangle$, $\overline{|\ a\rangle} \sim |\ \frac{1}{2}, -\frac{1}{2}\rangle$.

I will restrict my attention to the Raman process. This involves a two-phonon coupling through some other pair of levels $|\ b\rangle$ and $\overline{|\ b\rangle}$. The transition probability is given by

$$P = 2\pi \left| \sum_b \frac{\langle a \mid V_{k-} \mid b\rangle\langle b \mid V_{l+} \overline{|\ a\rangle}}{E_a - E_b + \omega_k} + \ldots \right|^2 \rho(E). \qquad (C.5)$$

The dots represent the three extra terms that arise when coupling to $\overline{|\ b\rangle}$ is introduced and the interactions are taken in the other order.

As the energy of the excited state $|\ b\rangle$ is much greater than the relevant phonon energies, it is a reasonable approximation to set the energy denominators to be equal. Now, if the interaction V is assumed to be time-even, then the terms in equation (C.5) approximately cancel due to the selection rule (C.4). This is just the well-known Van Vleck cancellation [Orbach and Stapelton 1972]. However, if we replace one of the operators in each term with a time-reversal odd interaction, this cancellation is avoided. Note that if we replace both interactions with time-odd ones, a Van Vleck cancellation reappears.

Thus the presence of time-odd interactions may be expected to have some effect on spin-lattice relaxation. To be able to experimentally distinguish time-odd effects from time-even ones, we need to find an experimental characteristic that is

qualitatively different for the two cases. As I will now show, a good candidate is the temperature dependence of the process.

That the time-odd and even processes will have different time-dependences follows from the following argument. Whatever the detailed mechanism may be, the time-odd ligand operator will be derived from a velocity and the time-even one from a position. Hence the time-reversal odd ligand operator will contain one more power of phonon frequency than the time-even one. Then, as the connection with temperature arises through an integral over frequency, we may expect qualitatively different time dependences for the two cases.

For time-even coupling to long-wavelength phonons, $V \sim \sqrt{\omega}$. A factor of ω comes from the fact that any relative motion or strain from acoustic phonons must be linear in wavevector and so frequency. The compensating $1/\sqrt{\omega}$ factor arises from the normalisation of the Fourier expansion of the strain operator in terms of normal mode amplitudes. Different frequency (and so time) dependences are observed for short-wavelength phonons [Shrivasata 1983].

For the time-odd case, we merely pick up an extra factor of ω due to the replacement of position coupling with momentum coupling. These two dependences may be verified by comparing the frequency dependence of the position and momentum operators for a simple harmonic oscillator. Hence time-reversal odd couplings should have at least one more power of temperature than time-even ones.

Many other phenomena, such as cross relaxation and phonon bottlenecks, can also lead to increased temperature dependences. For instance, in a site with inversion symmetry, the linear terms in the wavevector are inadequate to couple the odd modes of vibration. Nevertheless, these modes may be argued to still couple significantly at higher order in wavevector, and so with a correspondingly enhanced temperature dependence [Klimachev 1973]. Hence, any time-odd effect must be distinguished from the other mechanisms by which temperature dependence is enhanced.

For the Raman process discussed above, the time-even process has a T^9 tem-

perature dependence. Alternatively, magnetic field modulation of the ground state doublet leads to a weaker process with T^7B^2 dependence. Such dependences have been clearly verified experimentally [Pouw and van Duynevelkt 1976].

For the time-odd mechanism, the introduction of one time-odd interaction into each term of (C.5) avoids the Van Vleck cancellation with the associated factor of ω. However, the same factor is then reintroduced through the different frequency dependence of these matrix elements. Thus we must replace both interactions. Note that this leads to the reintroduction of the Van Vleck cancellation. Temperature dependences of T^{11} have been seen and variously explained in terms of time-even processes.

C.2.2 Reduction factors

The next example I will discuss is the Jahn-Teller reduction factors $K(\lambda)$ for the D_4 Jahn-Teller system. The effect of time-odd coupling on the Berry phases of this system has already been discussed in section 4.2. Reduction factors express the extent to which the matrix elements of an electronic operator (of a given point group symmetry λ) are reduced by lattice interaction with Jahn-Teller active modes.

In the absence of any time-odd coupling, these reduction factors obey sum rules. For example, the D_4 reduction factors obey the sum rule $2K(B_1) = 1 + K(A_2)$. We find that these rules are broken by the presence of time-reversal odd effects [Fletcher 1981]. Here I will give a simple perturbative proof.

In second quantisation, the Hamiltonian is given by (see equation (4.34))

$$\begin{aligned} H = {} & E(f_1^* f_1 + f_2^* f_2) + \omega_a(a^* a + \tfrac{1}{2}) + \omega_b(b_1^* b_1 + b_2^* b_2 + 1) \\ & + V_b\big((f_1^* f_1 - f_2^* f_2)(b_1 + b_1^*) + (f_1^* f_2 + f_2^* f_1)(b_2 + b_2^*)\big) \\ & + V_a(f_1^* f_2 - f_2^* f_1)(a - a^*). \end{aligned} \tag{C.6}$$

Here a^* creates a phonon in the A_2 mode, b_1^*, b_2^* create phonons in the B_1 and B_2 modes and f_1^*, f_2^* create electrons in the p_x and p_y states.

I will write the Hamiltonian eigenkets as $|\, in_a n_1 n_2\rangle$, these being derived by first order perturbation theory. The corresponding unperturbed states are written

$|\, in_a n_1 n_2\rangle_0$. Here the labels give the state of the electron and the number of quanta in each of the lattice modes.

It is a simple exercise in perturbation theory to calculate the following states:

$$|\, 1000\rangle = N\left(|\, 1000\rangle_0 + \frac{V_b}{\omega_b}(|\, 1010\rangle_0 + |\, 2001\rangle_0) + \frac{V_a}{\omega_b}|\, 2100\rangle_0\right), \quad (C.7)$$

$$|\, 2000\rangle = N\left(|\, 2000\rangle_0 + \frac{V_b}{\omega_b}(|\, 1001\rangle_0 - |\, 2010\rangle_0) - \frac{V_a}{\omega_a}|\, 1100\rangle_0\right), \quad (C.8)$$

where

$$N = \left(1 + \frac{2V_b^2}{\omega_b^2} + \frac{V_a^2}{\omega_a^2}\right)^{-1/2}. \quad (C.9)$$

Now the operators $f_1^* f_1 - f_2^* f_2$ and $f_1^* f_2 - f_2^* f_1$ are of symmetries B_1 and A_2 respectively. By direct substitution of equations (C.10) and (C.11), we find that

$$\langle 1000\,|\, f_1^* f_1 - f_2^* f_2\,|\, 1000\rangle = 1 - \frac{2V_b^2}{\omega_b^2} - \frac{V_a^2}{\omega_a 62}, \quad (C.10)$$

$$\langle 1000\,|\, f_1^* f_2 - f_2^* f_1\,|\, 2000\rangle = 1 - \frac{4V_b^2}{\omega_b^2}. \quad (C.11)$$

Further, the matrix elements with respect to the corresponding unperturbed states are both unity. Hence (C.13) and (C.14) are the reduction factors.

Now we have $2K(B_1) - 1 - K(A_2) = -2V_a^2/\omega_a^2$. Thus the time-odd coupling clearly has the effect of violating the sum rule $2K(B_1) = 1 + K(A_2)$. This violation competes with other sources of violation, such as the existence of a spectrum of lattice mode frequencies and contributions of fourth order in the ion-lattice coupling. Hence testing the validity of reduction factor sum rules is not a good way of looking for the effects of time-odd coupling.

C.2.3 Phonon Raman scattering

The final example I will discuss is phonon Raman spectroscopy. Here the formulation of phonon Raman scattering discussed by Churcher and Stedman [1981] is extended to include time-odd phonon coupling. By this is meant a Raman effect with photons of polarisation $\mathbf{e}$ and $\mathbf{e}'$ in which the electronic system eventually returns to the original level. Energy conservation is maintained by the emission of

a phonon in mode κk with energy $\omega_k = \omega - \omega'$. For convenience I write the labels in vector form: $\Omega = (\omega, \omega', \omega_k)$, $\overline{\Omega} = (\omega', \omega, -\omega_k)$, $s = (l, l', k)$ and $\overline{s} = (l', l, k)$.

Three interactions are involved so that equation (C.4) must be generalised accordingly. The Raman spectral feature has intensity

$$I_{\mathbf{e},\mathbf{e}'}(\Omega) = \sum_{s} \left| \sum_{\rho\rho'} e_\rho M_{ll'}^{\rho\rho'}(\Omega) e'_{\rho'} \right|^2 , \qquad (C.12)$$

where the relevant matrix elements $M_{ll'}^{\rho\rho'}$ are related to an effecive operator of the form

$$O^{\rho\rho'} = \sum_{\substack{M\mu N\nu \\ L''L'''}} \left(\langle L \mid D^\rho \mid M\mu \rangle \mid L'' \rangle \langle L'' \mid \langle M\mu \mid D^{\rho'} \mid N\nu \rangle \mid L''' \rangle \langle L''' \mid \right.$$
$$\left. \times \langle N\nu \mid V_k \mid L' \rangle / ((E_\Omega - E_M + \omega)(E_\Lambda - E_N - \omega')) + \ldots \right) (C.13)$$

The omitted terms correspond to the five alternative orderings of the three interactions (the electric dipole operator components D^ρ and $D^{\rho'}$ and the ion-lattice interaction V_k), with corresponding changes to the energy denominators.

In the equivalent denominator approximation, we obtain the selection rules

$$\mu \in [1 \otimes 1]_\eta, \qquad \nu \in [\Omega \otimes \Omega]_{\eta\tau_V\tau_\Lambda} \qquad \text{and} \qquad \mu^* \in \kappa \otimes \nu. \qquad (C.14)$$

Here μ is the coupling symmetry of the photon interactions, κ the phonon symmetry and ν a coupling symmetry for phonons and photons.

Applying these selection rules, we find that time-odd coupling allows new phonon modes to be Raman active [Moore and Stedman 1990a]. Note that symmetric phonons ($\kappa = 0$) are never Raman active for time-odd coupling within the states of a true irrep. This is because the characters of the symmetric irrep satisfy $\chi^0(g^2) = \chi^0(g)^2 = 1$. Thus the symmetric irrep is never present in the antisymmetric square of a true irrep.

On the face of it, breakthrough (Raman activation) of previously forbidden phonons would be a clear characterisation of time-odd coupling. As such it

competes against other sources of breakthrough. Notable among these are instrumental problems such as Snell's Law effects at boundaries [Lai *et al.* 1987] and a breakdown of the equivalent denominator approximation. Hence the best hope of detection of time-odd coupling through Raman scattering may rest with those phonon symmetries that are Raman active for both couplings, though in different polarisations.

Appendix D

Glossary

In this appendix, simple definitions of the most important technical terms used in this thesis are given.

almost everywhere: For a given σ-algebra there are many sets of measure ("size") zero, for example an isolated point on the real line. A property is said to hold almost everywhere if it is true except on a set of measure zero. Hence the function $y = x^2$ is non-zero almost everywhere, as it is non-zero except for the isolated point $x = 0$.

Berry phase: The overall phase for a given cyclic initial state can be written as the sum of two parts. The first is a geometrical property of the evolution and is called the Berry phase. The second is the time-integral of the instantaneous expectation value of the Hamiltonian. This is known as the dynamical phase.

Borel sets: *see* σ-algebra

bounded: An operator A is bounded if there exists a constant C such that $\|A\phi\| \leq C\|\phi\|$ for all vectors ϕ in the domain of A. The smallest such constant is called the norm of the operator. For example, all unitary operators are bounded with norm unity. This is because unitary operators preserve norms. An example of an unbounded operator is the position q. To see why, let ϕ_x be a normalised Gaussian wavepacket centred at x. Then $\|q\phi_x\|$ increases without bound as $x \to \infty$. A useful generalisation of the concept of boundedness is that of semi-boundedness. An operator A is semi-bounded if there exists a constant C such that $\langle\phi \mid A \mid \phi\langle \geq C\|\phi\|^2$ for all vectors ϕ in its domain of definition. The Hamiltonian of a harmonic oscillator is a good example of a semi-bounded (but not bounded) operator.

coherent state: Historically, coherent states were introduced as those states that behave as classically as possible. Since then the definition has been generalised and coherent states are generated by the action of a Lie group on a given initial state called the fiduciary state. The fiduciary state is often chosen to be the vacuum. A good example is provided by quantum optics. Here the output of a laser operating well above threshold is a particularly simple type of coherent state. These states are the eigenvectors of the boson annihilation operator and are usually called standard coherent states (see for example Perelomov [1986]).

connection: *see* holonomy.

cyclic initial space: A cyclic initial space is a subspace of the system's Hilbert space with the following property. All vectors in the space, when considered as initial states, evolve in such a way that the final state is also in the space. For example, the ray generated by a cyclic initial state is a cyclic initial space. Hence cyclic initial spaces are a true generalisation of cyclic initial states.

cyclic initial state: A cyclic initial state $\phi(0)$ for the $\tilde{t}$-periodic Hamiltonian $H(t)$ is a state that evolves in such a way that $\phi(\tilde{t}) = \exp\{i\chi\}\phi(0)$. These take the place of the eigenvectors used in the adiabatic case, allowing us to define non-adiabatic Berry phases. χ is called the overall phase.

dense: Let $\mathcal{H}$ be a Hilbert space and X be some subspace of $\mathcal{H}$. Then X is dense in $\mathcal{H}$ if any vector in $\mathcal{H}$ can be expressed as the limit of a sequence of elements in X. For example, the rational numbers are dense in the set of real numbers as every real number can be written as the limit of a sequence of rational numbers. In fact, this is often how the real numbers are defined!

domain: An unbounded self-adjoint operator cannot be defined on all of the Hilbert space. The set of vectors for which it is defined is called the domain of the operator. For example, the domain of the position operator q contains those vectors ϕ for which $q\phi$ is square-integrable.

dynamical phase: *see* Berry phase.

fibre bundle: A fibre bundle is a natural extension of the product $A \times B$ of two spaces. Subject to certain differentiability conditions, we require that the fibre bundle F can be locally written as a product. A simple example is the Möbius strip. This can locally be written as the product of a circle and a line segment. For this example the product representation is not local (the fibre bundle is not trivial) because of the twist in the strip. The most important fibre bundle in quantum mechanics is the Hopf bundle. This is locally the product of the projective Hilbert space and the group $U(1)$ of phases.

fiduciary state: *see* coherent state.

Floquet Hamiltonian: The dynamics for time-periodic Hamiltonians can be analysed by converting the problem into an equivalent time-independent form. The quantities of interest can then be found from the eigenvectors and eigenvalues of a certain operator called the Floquet Hamiltonian. This operator is calculated from the Fourier decomposition of the original Hamiltonian.

holonomy: Imagine that the quantum system of interest is following a certain path in the projective Hilbert space. To describe the system in the full Hilbert space, we have to "provide a phase". The choice of this phase is called a connection. There is a natural connection induced by the inner product structure of the Hilbert space. If our path in projective Hilbert space starts and ends at the same point (we start in a cyclic initial state), then the total phase change generated by the connection is called the holonomy. It turns out that the holonomy of the natural connection is just the Berry phase. Some authors prefer the term "anholonomy" to holonomy (for example Berry [1990b]). This usage derives from the mechanics of systems subject to constraints. The constraint is called holonomic if it is integrable and anholonomic otherwise. As the non-triviality of the Berry phase is due to its non-integrability, it seems natural to describe it as an anholonomy.

Jaynes-Cummings model: The Jaynes-Cummings model describes the Hamiltonian of a two-level atom in a semi-classical radiation field in the rotating wave

approximation. This situation can be realised to a good approximation by subjecting an atom to an intense radiation field that is nearly in resonance with one of its atomic transitions.

monodromy operator: Let $U(t)$ be the evolution operator corresponding to the $\tilde{t}$-periodic Hamiltonian $H(t)$. Then $U(\tilde{t})$, the evolution operator at the end of one period, is called the monodromy operator. This is because $U(\tilde{t})$ generates the long-term evolution of the system; $U(n\tilde{t}+t) = U(\tilde{t})^n U(t)$.

normal: An operator A is normal if $AA^* = A^*A$. Both self-adjoint and unitary operators are normal.

overall phase: *see* cyclic initial state.

quasi-energy: The analysis of systems with periodic Hamiltonians $H(t)$ can be reduced to an equivalent "time-independent" form by using the Floquet Hamiltonian $K = H - \mathrm{i}\frac{\partial}{\partial t}$. The eigenvectors of this Hamiltonian are closely related to the cyclic initial states and are called quasi-energy states. The corresponding eigenvalues are called quasi-energies.

reduced density operator: The state of a quantum system can be described by a density operator ρ, the expectation value of the observable A being given by $\mathrm{Tr}(\rho A)$. In many situations however, we are only interested in a certain part of the whole system. For example, in modelling a laser, the system contains atomic and photon degrees of freedom. It is only the photon degrees of freedom that matter in calculating the statistics of the laser output. To get rid of the atomic variables, all we need to do is trace them out of the density operator. This gives a reduced density operator which enables the expectation values of the photon observables to be efficiently calculated. This approach is often used to couple a system of interest to its surroundings, such as a heat bath.

self-adjoint: An operator is self-adjoint if it is equal to its adjoint. I use this term rather than "hermitian" as some mathematicians use hermitian to mean "symmetric". An operator A is symmetric if $\langle A\phi \mid \psi\rangle = \langle \phi \mid A\psi\rangle$ for all vectors

ϕ and ψ in its domain of definition. While the concepts of self-adjointness and symmetry are the same for bounded operators, they are not for unbounded ones.

σ-algebra: To define integration rigorously, one needs to define the "size" of a set. However it turns out that size cannot be defined in a consistent way for all of the subsets of the integration range. The set of measurable sets must satisfy certain technical conditions in order that the resulting integral have properties such as linearity. These conditions define a σ-algebra. For the real line, we obviously want the open intervals (a, b) to be measurable with measure $b - a$. The sets in the resulting σ-algebra are called Borel sets. The Borel sets define the standard Lebesgue integral.

single-valued vector: Let $\phi(0)$ be a cyclic initial state for the Hamiltonian $H(t)$. Then $\phi(\tilde{t}) = \exp\{i\chi\}\phi(0)$. A single-valued vector is any state $\psi(t)$ of the form $\psi(t) = \exp\{i\theta(t)\}\phi(t)$ satisfying $\psi(\tilde{t}) = \psi(0)$. These vectors are used to calculate the Berry phase for the initial state $\phi(0)$ and allow a unified treatment of the various calculational methods used in the literature.

spectral measure: On a finite-dimensional Hilbert space, any self adjoint operator A can be written in the form $A = \sum a_n P_n$. Here a_n is an eigenvalue and P_n is the orthogonal projector onto the corresponding eigenspace. This is not possible in general for systems with infinite dimensional Hilbert spaces due to the presence of a continuous part of the spectrum. However a similar expression, where we integrate over the spectrum does exist. This integration uses an operator extension of the concept of measure used in normal integration theory. This generalisation is called a spectral measure.

spectrum: The spectrum of an operator A is the set of those complex numbers λ for which $\lambda - A$ is not invertible. The spectrum contains the eigenvalues of the operator as well as a continuous part.

unitary: An operator is unitary if it maps one basis of the Hilbert space onto another. This is equivalent to requiring that its inverse be its adjoint. Unitary operators are bounded with norm unity.

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